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Fire Dynamics Simulator (Version 5) User's Guide

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In cooperation with:
VTT Technical Research Centre of Finland

NIST

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Preface

This Guide describes how to use the Fire Dynamics Simulator (FDS) version 5. Because new features are added periodically, check the current version number on the inside front jacket of this manual.

Note that this Guide does not provide the background theory for FDS. A four volume set of companion documents, referred to collectively as the FDS Technical Reference Guide [1], contains details about the governing equations and numerical methods, model verification, experimental validation, and configuration management. The FDS User's Guide contains limited information on how to operate Smokeview, the companion visualization program for FDS. Its full capability is described in the Smokeview User's Guide [2].

Disclaimer

The US Department of Commerce makes no warranty, expressed or implied, to users of the Fire Dynamics Simulator (FDS), and accepts no responsibility for its use. Users of FDS assume sole responsibility under Federal law for determining the appropriateness of its use in any particular application; for any conclusions drawn from the results of its use; and for any actions taken or not taken as a result of analyses performed using these tools.

Users are warned that FDS is intended for use only by those competent in the fields of fluid dynamics, thermodynamics, combustion, and heat transfer, and is intended only to supplement the informed judgment of the qualified user. The software package is a computer model that may or may not have predictive capability when applied to a specific set of factual circumstances. Lack of accurate predictions by the model could lead to erroneous conclusions with regard to fire safety. All results should be evaluated by an informed user.

Throughout this document, the mention of computer hardware or commercial software does not constitute endorsement by NIST, nor does it indicate that the products are necessarily those best suited for the intended purpose.

About the Authors

Kevin McGrattan is a mathematician in the Building and Fire Research Laboratory of NIST. He received a bachelors of science degree from the School of Engineering and Applied Science of Columbia University in 1987 and a doctorate at the Courant Institute of New York University in 1991. He joined the NIST staff in 1992 and has since worked on the development of fire models, most notably the Fire Dynamics Simulator.

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Acknowledgments

The Fire Dynamics Simulator, in various forms, has been under development for almost 25 years. However, the publicly released software has only existed since 2000. Since its first release, continued improvements have been made to the software based largely on feedback from its users. Included here are some who made important contributions.

At NIST, thanks to Dan Madrzykowski, Doug Walton, Bob Vettori, Dave Stroup, Steve Kerber and Nelson Bryner, who have used FDS and Smokeview as part of several investigations of fire fighter line of duty deaths. As part of these studies, they have provided valuable information on the model's usability and accuracy when compared to large scale measurements made during fire reconstructions.

Bryan Klein of NIST assisted in adding cross-referencing functionality to this document, making it easier to view electronically.

The US Nuclear Regulatory Commission has provided financial support for the maintenance and development of FDS, along with valuable insights into how fire models are used as part of probabilistic risk assessments of nuclear facilities. Special thanks to Mark Salley and Jason Dreisbach of NRC, and Francisco Joglar of SAIC.

The Society of Fire Protection Engineers (SFPE) sponsors a training course on the use of FDS and Smokeview. Chris Wood of ArupFire, Dave Sheppard of the US Bureau of Alcohol, Tobacco and Firearms (ATF), and Doug Carpenter of Combustion Science and Engineering developed the materials for the course, along with Morgan Hurley of the SFPE.

Prof. David McGill of Seneca College, Ontario, Canada has conducted a remote-learning course on the use of FDS, and he has also maintained a web site that has provided valuable suggestions from users.

Prof. Ian Thomas of Victoria University has also presented short courses on the use of FDS in Australia. His students have also performed some validation work on compartment fires.

Prof. Charles Fleischmann and his students at the University of Canterbury, New Zealand, have provided valuable assistance in improving the documentation and usability of the model.

James White Jr. of the Western Fire Center has provided valuable feedback on how to improve the functionality of the model in the area of forensic science.

Paul Hart of Swiss Re, GAP Services, and Pravinray Gandhi of Underwriters Laboratories provided useful suggestions about water droplet transport on solid objects.

Dr. Chris Lautenberger of University of California, Berkeley, has helped in development and improving the documentation of the pyrolysis models.

Finally, on the following pages is a list of individuals and organizations who have volunteered their time and effort to "beta test" FDS and Smokeview prior to its official release. Their contribution is invaluable because there is simply no other way to test all of the various features of the model.

FDS 5 Beta Testers	
Nick Agnew	Maunsell, Australia
Camille Azzi	Universities of Glasgow and Strathclyde, Scotland
Matthew Bilson	Maunsell, Australia
George Braga	Federal District Fire Department, Brazil
Keith Calder	Senez Reed Calder Engineering, Canada
Steven Chi Heng Lam	Hoare Lea Fire Engineering, UK
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Marco Cigolini	Italferr spa, Italy
John Cutonilli	Hughes Associates, Inc., USA
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Franck Didieux	Laboratoire National de Métrologie et d'Essais (LNE), France
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Paul Fuss	NIST, USA
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Andreas Gerndt	University of Louisiana, USA
Emanuele Gissi	Corpo Nazionale dei Vigili del Fuoco, Comando Prov. di Genova, Italy
Simon J. Ham	Fire Safety Engineering Consultants Ltd., UK
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Pierre-Louis Lamballais	Flashover-Backdraft, France
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Davy Leroy	Arup Fire, UK
Yunlong Liu	Parsons Brinckerhof, Australia
Timothy Liu	Locke Carey Fire Consultants, UK
Dave McGill	Seneca College, Ontario, Canada
Ken Miller	Las Vegas Fire & Rescue, USA
Stephan B. Miller	Mr. 3D Computer Graphics and the University of Houston Downtown, USA
Pete Muir	Safe Consulting, UK
Stephen Olenick	Combustion Science & Engineering, Inc., USA
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Part I

The Basics of FDS

Chapter 1

Introduction

The software described in this document, Fire Dynamics Simulator (FDS), is a computational fluid dynamics (CFD) model of fire-driven fluid flow. FDS solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. The formulation of the equations and the numerical algorithm are contained the FDS Technical Reference Guide [1].

Smokeview is a separate visualization program that is used to display the results of an FDS simulation. A detailed description of Smokeview is found in a separate user's guide [2].

1.1 Features of FDS

The first version of FDS was publicly released in February 2000. To date, about half of the applications of the model have been for design of smoke handling systems and sprinkler/detector activation studies. The other half consist of residential and industrial fire reconstructions. Throughout its development, FDS has been aimed at solving practical fire problems in fire protection engineering, while at the same time providing a tool to study fundamental fire dynamics and combustion.

Hydrodynamic Model FDS solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow with an emphasis on smoke and heat transport from fires. The core algorithm is an explicit predictor-corrector scheme, second order accurate in space and time. Turbulence is treated by means of the Smagorinsky form of Large Eddy Simulation (LES). It is possible to perform a Direct Numerical Simulation (DNS) if the underlying numerical mesh is fine enough. LES is the default mode of operation.

Combustion Model For most applications, FDS uses a single step chemical reaction whose products are tracked via a two-parameter mixture fraction model. The mixture fraction is a conserved scalar quantity that represents the mass fraction of one or more components of the gas at a given point in the flow field. By default, two components of the mixture fraction are explicitly computed. The first is the mass fraction of unburned fuel and the second is the mass fraction of burned fuel (*i.e.* the mass of the combustion products that originated as fuel). A two-step chemical reaction with a three parameter mixture fraction decomposition can also be used with the first step being oxidation of fuel to carbon monoxide and the second step the oxidation of carbon monoxide to carbon dioxide. The three mixture fraction components for the two step reaction are unburned fuel, mass of fuel that has completed the first reaction step, and the mass of fuel that has completed the second reaction step. The mass fractions of all of the major reactants and products can be derived from the mixture fraction parameters by means of "state relations." Lastly, a multiple-step finite rate model is also available.

Radiation Transport Radiative heat transfer is included in the model via the solution of the radiation transport equation for a gray gas, and in some limited cases using a wide band model. The equation is solved using a technique similar to finite volume methods for convective transport, thus the name given to it is the Finite Volume Method (FVM). Using approximately 100 discrete angles, the finite volume solver requires about 20 % of the total CPU time of a calculation, a modest cost given the complexity of radiation heat transfer. The absorption coefficients of the gas-soot mixtures are computed using RADCAL narrow-band model. Liquid droplets can absorb and scatter thermal radiation. This is important in cases involving mist sprinklers, but also plays a role in all sprinkler cases. The absorption and scattering coefficients are based on Mie theory.

Geometry FDS approximates the governing equations on a rectilinear mesh. Rectangular obstructions are forced to conform with the underlying mesh.

Multiple Meshes This is a term used to describe the use of more than one rectangular mesh in a calculation. It is possible to prescribe more than one rectangular mesh to handle cases where the computational domain is not easily embedded within a single mesh.

Parallel Processing It is possible to run an FDS calculation on more than one computer using the Message Passing Interface (MPI). Details can be found in Section 3.1.2.

Boundary Conditions All solid surfaces are assigned thermal boundary conditions, plus information about the burning behavior of the material. Heat and mass transfer to and from solid surfaces is usually handled with empirical correlations, although it is possible to compute directly the heat and mass transfer when performing a Direct Numerical Simulation (DNS).

1.2 What's New in FDS 5?

FDS 5 differs from previous versions in its treatment of solid boundaries and gas phase combustion. Among the more important changes are:

Multi-Step Combustion Previous versions of FDS have assumed only one gas phase reaction. Now, multiple-step reaction schemes are available to describe local extinction, CO production, among various other phenomena. The most important improvements to the combustion model are a more accurate heat release rate calculation, and a better treatment of local flame extinction.

Material Layers Past versions of FDS have assumed that solid boundaries consist of a single homogenous layer. Now, solid boundaries can be modeled with multiple layers of materials, with each material specified via a new namelist group called `MATL`. This change makes past input files obsolete.

Command Line Format FDS is still run from the command line, but the syntax is slightly different than in previous versions. See Section 3 for details.

Database Previous versions of FDS used a separate "database" file to store material and reaction parameters. This file is no longer available, and now all parameters must be specified within the input file.

Device Descriptions The method used to describe a device and/or sensor (Sprinkler, Heat Detector, Thermocouple, etc.) has changed. See Section 13.1 for more information on defining devices and their properties. Any device can be used to control sprinkler activation and the creation and removal of vents or obstacles.

Sprinklers The external sprinkler files used in previous versions are no longer used. All information about sprinklers and other fire-specific devices are conveyed in the input file. Sprinklers are now defined with the new method of describing devices mentioned above. See Section 13.1 for more information.

Control Functions A new group of input parameters is available to describe functions that control sprinkler activation, the creation and removal of vents or obstacles, and code execution (termination or dumping of restart files). See Section 13.5 for details.

Numerical Mesh Previous versions of FDS used separate input groups to define the numerical grid and the computational domain. Now the two groups have been merged into a single, simplified `MESH` namelist group. Namelist groups `PDIM` and `GRID` shall no longer be used in the input file. See Section 6.3 for more detail.

Pressure Zones It is possible in FDS 5 to declare individual regions in the computational domain to have background pressures different from ambient, allowing for calculations of leakage, fan curves, and so forth. See Section 9.6 for more details.

Stack Effect and Atmospheric Stratification Improvements have been made to better characterize a stratified atmosphere and the movement of air in a tall building due to temperature differences between inside and outside.

Adiabatic Surface Temperature A new output quantity has been added to facilitate using FDS output in thermal and mechanical finite element models. See Section 8.1.1 for more information.

Development, Distribution and Formal User Support Starting with FDS 5, an online, open-source development environment is being used for configuration management (code archiving, revision tracking, bug fixes, user suggestions, and so on). See Section 2.1 for more information.

FDS Verification and Validation Information Starting with FDS 5, more emphasis has been placed on maintaining a permanent collection of Verification and Validation cases. This improves the quality of each FDS update and release, as a standard test suite will now be used to insure that changes made to the source code do not degrade FDS output. This also provides users with a standard data set to verify their own installation of FDS and to compare the results that FDS is returning on their system to published data.

Chapter 2

Getting Started

FDS is a computer program that solves equations that describe the evolution of fire. It is a Fortran program that reads input parameters from a text file, computes a numerical solution to the governing equations, and writes user-specified output data to files. Smokeview is a companion program that reads FDS output files and produces animations on the computer screen. Smokeview has a simple menu-driven interface. FDS does not. However, there are various third-party programs that have been developed to generate the text file containing the input parameters needed by FDS.

This guide describes how to obtain FDS and Smokeview and how to use FDS. A separate document [2] describes how to use Smokeview. Other tools related to FDS and Smokeview can be found at the web site.

2.1 How to Acquire FDS and Smokeview

Detailed instructions on how to download executables, manuals, source-code and related utilities, can be found on the FDS-SMV Website `http://fire.nist.gov/fds`. The typical FDS/Smokeview distribution consists of an installation package or compressed archive, which is available for MS Windows, Mac OS X, and Linux. For other operating systems, consult the web site.

> If you ever want to keep an older version of FDS and Smokeview, copy the installation directory to some other place so that it is not overwritten during the updated installation.

2.2 Computer Hardware Requirements

FDS requires a fast CPU[1] and a substantial amount of random-access memory (RAM) to run efficiently. For minimum specifications, the system should have a 1 GHz CPU, and at least 512 MB RAM. The CPU speed will determine how long the computation will take to finish, while the amount of RAM will determine how many mesh cells can be held in memory. A large hard drive is required to store the output of the calculations. It is not unusual for the output of a single calculation to consume more than 1 GB of storage space.

Most computers purchased within the past few years are adequate for running Smokeview with the caveat that additional memory (RAM) should be purchased to bring the memory size up to at least 512 MB. This is so the computer can display results without "swapping" to disk. For Smokeview it is also important to obtain a fast graphics card for the PC used to display the results of the FDS computations.

For Multi-Mesh calculations, the MPI version of FDS will operate over standard 100 Mbps networks. A Gigabit or 1000 Mbps network will further reduce latency and improve data transfer rates between nodes.

---

[1]Central Processing Unit

2.3 Computer Operating System (OS) and Software Requirements

The goal of making FDS and Smokeview publicly available has been to enable practicing fire protection engineers to perform fairly sophisticated fire simulations at a reasonable cost. Thus, FDS and Smokeview have been designed for computers running Microsoft Windows, Mac OS X, and various implementations of Unix/Linux.

MS Windows An installation package is available for Windows operating system. It is not recommended to run FDS/Smokeview under any version of MS Windows released prior to Windows 2000.

Mac OS X A zip archive is available for Intel architectures. Mac OS X 10.4.x or better is recommended, versions of OS X prior to 10.4.x are not officially supported. Users can always download the latest version of FDS source and compile FDS for other versions of OS X (See Appendix 18 for details).

Linux Pre-compiled executables are available that can be installed in an appropriate directory. Note that the installation package is simply an archive and no path variables are set. If the pre-compiled FDS executable does not work (usually because of library incompatibilities), the FDS source code can be downloaded and compiled using a Fortran 90 and C compiler (See Appendix 18 for details). If Smokeview does not work on the Linux workstation, you can use the Windows version to view FDS output.

Unix There are no pre-compiled versions of FDS for the various flavors of Unix. However, the advice for Linux applies equally as well to Unix.

FDS in Parallel For those wishing to run FDS in parallel, MPI (Message Passing Interface) must be installed on each of the computers within the network that will be used for FDS computations. Information about installing MPI on different computer platforms is given on the FDS website. See the Development section of the website for more information.

Chapter 3

Running FDS

This chapter describes the procedure to run an FDS calculation. The primary requirement for any calculation is an FDS input file. The creation of an input file is covered in detail in Part II. If you are new to FDS and Smokeview, it is strongly suggested that you start with an existing data file, run it as is, and then make the appropriate changes to the input file for the desired scenario. Sample input files are included as part of the standard installation. By running a sample case, you become familiar with the procedure, learn how to use Smokeview, and ensure that your computer is up to the task before embarking on learning how to create new input files.

3.1 Starting an FDS Calculation

FDS can be run from the command prompt, or with a third party Graphical User Interface (GUI). In the discussion to follow, it is assumed that FDS is being run from the command prompt. FDS can be run on a single computer, using only one CPU, or it can be run on multiple computers and use multiple CPUs. For any operating system, there are two FDS executable files. The single CPU Windows executable is called **fds5.exe**. The parallel executable is called **fds5_mpi.exe**. The letters "mpi" in the filename denote Message Passing Interface (MPI), which will be discussed below.

> Note that the input file for both single and parallel versions of FDS are the same. In fact, it is recommended that before embarking on parallel processing, you should run your input file in serial mode to ensure that it is properly set up.

3.1.1 Starting an FDS Calculation (Single Processor Version)

Sample input files are provided with the program for new users who are encouraged to first run a sample calculation before attempting to write an input file. Assuming that an input file called **job_name.fds** exists in some directory, run the program either in a DOS or Unix command prompt as follows:

MS Windows

Open up a Command Prompt window (click Start, then Run, then type "cmd"), and change directories ("cd") to where the input file for the case is located, then run the code by typing at the command prompt

```
fds5 job_name.fds
```

The character string `job_name` is usually designated within the input file as the `CHID`. It is recommended that the name of the input file and the `CHID` be the same so that all of the files associated with a given calculation have a consistent name. The progress of a simulation is indicated by diagnostic output that is written out onto the screen. Detailed diagnostic information is automatically written to a file **CHID.out**, where `CHID` is a character string, usually the same as `job_name`, designated in the input file.. Screen output can be redirected to a file via the alternative command

```
fds5 job_name.fds > job_name.err
```

Note that it is also possible to associate the extention "fds" with the FDS executable directly, thereby making FDS run by double-clicking on the input file. If you do this, note that error messages will be written to the .out file. Also, if you associate the input file with the FDS executable, be careful not to accidently double-click on the input file when trying to edit it. This action will cause previously generated output files to be over-written.

Mac OS X, Unix, Linux

Depending on the type of installation, you may need to set various path or environment variables in order to invoke FDS without a full path reference to the executable. The easiest way to do this is via an "alias" in your shell start-up script. For the example below, it is assumed that `fds5` is aliased to its full path name. You may also need to "chmod + x" to make the file executable. Once this is done, run FDS from the command line by typing:

```
fds5 job_name.fds
```

The input parameters are read from the file **job_name.fds**, and error statements and other diagnostics are written out to the screen. To run the job in the background:

```
fds5 job_name.fds >& job_name.err &
```

Note that in the latter case, the screen output is stored in the file **job_name.err** and the detailed diagnostics are saved automatically in a file **CHID.out**, where `CHID` is a character string, usually the same as `job_name`, designated in the input file. It is preferable to run jobs in the background so as to free the console for other uses.

3.1.2 Starting an FDS Calculation (Multiple Processor Version)

Running FDS across a network using multiple processors and multiple banks of memory (RAM) is more difficult than running the single processor version. More is required of the user to make the connections between the machines as seamless as possible. This involves creating accounts for a given user on each machine, sharing directories, increasing the speed of the network, making each machine aware of the others, *etc.* Some of these details are handled by the parallel-processing software, others are not. Undoubtedly the procedure will be simplified in years to come, but for the moment, parallel-processing is still relatively new and requires more expertise in terms of understanding both the operating system and the network connections of a given set of computers.

FDS uses MPI (Message-Passing Interface) [3] to allow multiple computers to run a single FDS job. The main idea is that you must break up the FDS domain into multiple meshes, and then the flow field in each mesh is computed as a different *process*. Note the subtle difference between these terms – a *process* does not have the same meaning as a *processor*. The *process* can be thought of as a "task" that you would see in the Windows Task Manager or by executing the "top" command on a Linux/Unix machine. The *processor* refers to the computer hardware. A single *processor* may run multiple *processes*, for example. The computation

on a given FDS mesh is thought of as an individual *process*, and MPI handles the transfer of information between these *processes*. Usually, each mesh is assigned its own *process* in a parallel calculation, although it is also possible assign multiple meshes to a single *process*.[1] In this way, large meshes can be computed on dedicated *processors*, while smaller meshes can be clustered together in a single *process* running on a single *processor*, without the need for MPI message passing between themselves.

Also note that FDS refers to its meshes by the numbers 1, 2, 3, and so on, whereas MPI refers to its processes by the numbers 0, 1, 2, and so on. Thus, Mesh 1 is assigned to Process 0; Mesh 2 to Process 1, and so on. As a user, you never actually number the meshes or the processes yourself, but error statements from FDS or from MPI might refer to the meshes or processes by number. As an example, if a five mesh FDS case is run in parallel, the first printout (usually to the screen unless otherwise directed) is:

```
Process  4 of  4 is running on fire65
Process  3 of  4 is running on fire64
Process  2 of  4 is running on fire63
Process  0 of  4 is running on fire61
Process  1 of  4 is running on fire62
Mesh   1 is assigned to Process   0
Mesh   2 is assigned to Process   1
Mesh   3 is assigned to Process   2
Mesh   4 is assigned to Process   3
Mesh   5 is assigned to Process   4
```

This means that 5 processes (numbered 0 to 4) have started on the computers named fire61, fire62, *etc.*, and that each mesh is being computed as an individual process on the individual computers. Each computer has its own memory (RAM), and MPI is the protocol by which information is passed from process to process during the calculation. Note that these computers may have multiple processors, and each processor may have multiple "cores." You have control over how many processes get assigned to each computer, but you may or may not have control over how the processes are handled by a given computer. That depends on the operating system and the particular version of MPI. For example, fire62 happens to have two quad-core processors, and all five meshes could have been assigned to run as five processes all on fire62. Whether or not this is the best strategy is still a subject of research and heavily dependent on the technical specifications of the OS and hardware.

There are different implementations of MPI, much like there are different Fortran and C compilers. Each implementation is essentially a library of subroutines called from FDS that transfer data from one thread to another across a fast network. The format of the subroutine calls has been widely accepted in the community, allowing different vendors and organizations the freedom to develop better software while working within an open framework.

The way FDS is executed in parallel depends on which implementation of MPI has been installed. At NIST, the parallel version of FDS is presently run on Windows PCs connected by the Local Area Network (LAN, 100 Mbps) or on a cluster of Linux PCs linked together with a dedicated, fast (1000 Mbps) network. The Windows computers use MPICH2, a free implementation of MPI from Argonne National Laboratory, USA.

MPICH2

With MPICH2, a parallel FDS calculation can be invoked either from the command line or by using a Graphical User Interface (GUI). After the MPICH2 libraries are installed on each computer and the necessary directories are shared, FDS is run using the command issued from one of the computers

---

[1]Assigning multiple meshes to a single process was introduced in FDS version 5.3.

```
mpiexec -file config.txt
```

where **config.txt** is a text file containing the name and location of the FDS executable, name of the FDS input file, the working directory, and the names of the various computers that are to run the job. For example, the **config.txt** file might look like this for a job run at NIST with computers named fire_1, fire_2, and fire_3:

```
exe \\fire_1.nist.gov\NIST\FDS\fds5_mpi.exe job_name.fds
dir \\fire_1.nist.gov\Projects\
hosts
fire_1.nist.gov 2
fire_2.nist.gov 1
fire_3.nist.gov 2
```

The numbers following the "host" machines represent the number of threads to run on that particular machine. In this example, 5 threads are run for an FDS calculation that has 5 meshes. The `exe` and `dir` directories need to be shared, with the latter having read and write permissions.

All the computers must be able to access the executable and the working directory on `fire_1`. This is achieved under Windows by "sharing." Under Unix/Linux and OS X, the process involves cross-mounting the file systems of the various machines.

LAM-MPI

On the Linux cluster in the Building and Fire Research Lab at NIST, LAM-MPI, a free implementation from Indiana University, is installed.[2] With LAM/MPI, the computers to be used are linked prior to the actual execution of FDS with a separate command called a "lamboot." FDS is then run using the command

```
mpirun -np 5 fds5_mpi job_name.fds
```

where the 5 indicates that 5 processors are to be used. In this case, the executable **fds5_mpi** is located in the working directory. To make the process run in the background

```
mpirun -np 5 fds5_mpi job_name.fds >& job_name.err &
```

The file **job_name.err** contains what is normally printed out to the screen.

Note that there are several other implementations of MPI, some free, some not. Support for the software varies, thus FDS has been designed to run under any of the more popular versions without too much user intervention. However, keep in mind that parallel processing is a relatively new area of computer science, and there are bound to be painful growth spurts in the years ahead.

3.2 Monitoring Progress

Diagnostics for a given calculation are written into a file called **CHID.out**. The CPU usage and simulation time are written here, so you can see how far along the program has progressed. At any time during a calculation, Smokeview can be run and the progress can be checked visually. To stop a calculation before its scheduled time, either kill the process, or preferably create a file in the same directory as the output files

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[2]http://www.lam-mpi.org

called **CHID.stop**. The existence of this file stops the program gracefully, causing it to dump out the latest flow variables for viewing in Smokeview.

Since calculations can be hours or days long, there is a restart feature in FDS. Details of how to use this feature are given in Section 6.4.2. Briefly, specify at the beginning of calculation how often a "restart" file should be saved. Should something happen to disrupt the calculation, like a power outage, the calculation can be restarted from the time the last restart file was saved.

It is also possible to control the stop time and the dumping of restart files by using control functions as described in Section 13.5.

Chapter 4

User Support

It is not unusual over the course of a project to run into various problems, some related to FDS, some related to your computer. FDS is not a typical PC application. It is a serious calculation that pushes your computer's processor and memory to its limits. In fact, there are no hardwired bounds within FDS that prevent you from starting a calculation that is too much for your hardware. Even if your machine has adequate memory (RAM), you can still easily set up calculations that can require weeks or months to complete. It is difficult to predict at the start of a simulation just how long and how much memory will be required. Learn how to monitor the resource usage of your computer. Start with small calculations and build your way up.

Although many features in FDS are fairly mature, there are many that are not. FDS is used for practical engineering applications, but also for research in fire and combustion. As you become more familiar with the software, you will inevitably run into areas that are of current research interest. Indeed, burning a roomful of ordinary furniture is one of the most challenging applications of the model. So be patient, and learn to dissect a given scenario into its constitutive parts. For example, do not attempt to simulate a fire spreading through an entire floor of a building unless you have simulated the burning of the various combustibles with relatively small calculations.

Along with the FDS User's Guide, there are resources available on the Internet. These include an "Issue Tracker," that allows you to report bugs, request new features, and ask specific clarifying questions, and "Group Discussions," which support more general topics than just specific problems. Before using these on-line resources, it is important to first try to solve your own problems by performing simple test calculations, or debugging your input file. The next few sections provide a list of error statements and suggestions on how to solve problems.

4.1 The Version Number

If you encounter problems with FDS, it is crucial that you submit, along with a description of the problem, the FDS version number. Each release of FDS comes with a version number like 5.2.6, where the first number is the *major* release, the second is the *minor* release, and the third is the *maintenance* release. Major releases occur every few years, and as the name implies dramatically change the functionality of the model. Minor releases occur every few months, and may cause minor changes in functionality. Release notes can help you decide whether the changes should effect the type of applications that you typically do. Maintenance releases are just bug fixes, and should not affect code functionality. To get the version number, just type the executable at the command prompt:

```
fds5
```

and the relevant information will appear, along with a date of compilation (useful to you) and a so-called SVN number (useful to us). The SVN number refers to the Subversion repository number of the source code. It allows us to go back in time and recover the exact source code files that were used to build that executable.

Simply get in the habit of checking the version number of your executable, periodically checking for new releases which might already have addressed your problem, and telling us what version you are using if you report a problem.

4.2   Common Error Statements

An FDS calculation may end before the specified time limit. Following is a list of common error statements and how to diagnose the problems:

Input File Errors: The most common errors in FDS are due to mis-typed input statements. These errors result in the immediate halting of the program and a statement like, "ERROR: Problem with the HEAD line." For these errors, check the line in the input file named in the error statement. Make sure the parameter names are spelled correctly. Make sure that a / (forward slash) is put at the end of each namelist entry. Make sure that the right type of information is being provided for each parameter, like whether one real number is expected, or several integers, or whatever. Make sure there are no non-ASCII characters being used, as can sometimes happen when text is cut and pasted from other applications or word-processing software. Make sure zeros are zeros and O's are O's. Make sure 1's are not !'s. Make sure apostrophes are used to designate character strings. Make sure the text file on a Unix/Linux machine was not created on a DOS machine, and *vice versa*. Make sure that all the parameters listed are still being used – new versions of FDS often drop or change parameters to force you to re-examine old input files.

Numerical Instability Errors: It is possible that during an FDS calculation the flow velocity at some location in the domain can increase due to numerical error causing the time step size to decrease to a point where logic in the code decides that the results are unphysical and stops the calculation with an error message in the file **CHID.out**. In these cases, FDS ends by dumping out one final Plot3D file giving the user some means by which to see where the error is occurring within the computational domain. Usually, a numerical instability can be identified by fictitiously large velocity vectors emanating from a small region within the domain. Common causes of such instabilities are mesh cells that have an aspect ratio larger than 2 to 1, high speed flow through a small opening, a sudden change in the heat release rate, or any number of sudden changes to the flow field. There are various ways to solve the problem, depending on the situation. Try to diagnose and fix the problem before reporting it. It is difficult for anyone but the originator of the input file to diagnose the problem.

Inadequate Computer Resources: The calculation might be using more RAM than the machine has, or the output files could have used up all the available disk space. In these situations, the computer may or may not produce an intelligible error message. Sometimes the computer is just unresponsive. It is your responsibility to ensure that the computer has adequate resources to do the calculation. Remember, there is no limit to how big or how long FDS calculations can be – it depends on the resources of the computer. For any new simulation, try running the case with a modest-sized mesh, and gradually make refinements until the computer can no longer handle it. Then back off somewhat on the size of the calculation so that the computer can comfortably run the case. Trying to run with 90 % to 100 % of computer resources is risky. In fact, for a typical 32 bit Windows PC with 4 GB RAM, only 2 GB will be available to FDS, based on user feedback. If you want to run bigger cases, consider buying a computer with a 64 bit operating system or break up the calculation into multiple meshes and use parallel processing.

Run-Time Errors: An error occurs either within the computer operating system or the FDS program. An error message is printed out by the operating system of the computer onto the screen or into the diagnostic output file. This message is most often unintelligible to most people, including the programmers, although occasionally one might get a small clue if there is mention of a specific problem, like "stack overflow," "divide by zero," or "file write error, unit=..." These errors may be caused by a bug in FDS, for example if a number is divided by zero, or an array is used before it is allocated, or any number of other problems. Before reporting the error to the Issue Tracker, try to systematically simplify the input file until the error goes away. This process usually brings to light some feature of the calculation responsible for the problem and helps in the debugging.

File Writing Errors: Occasionally, especially on Windows machines, FDS fails because it is not permitted to write to a file. A typical error statement reads:

```
forrtl: severe (47): write to READONLY file, unit 8598, file C:\Users\...\
```

The unit, in this case 8598, is just a number that FDS has associated with one of the output files. If this error occurs just after the start of the calculation, you can try adding the phrase
`FLUSH_FILE_BUFFERS=.FALSE.`
on the `DUMP` line of the input file (see Section 14.1). This will prevent FDS from attempting to flush the contents of the internal buffers, something it does to make it possible to view the FDS output in Smokeview during the FDS simulation.

Poisson Initialization: Sometimes at the very start of a calculation, an error appears stating that there is a problem with the "Poisson initialization." The equation for pressure in FDS is known as the Poisson equation. The Poisson solver consists of large system of linear equations that must be initialized at the start of the calculation. Most often, an error in the initialization step is due to a mesh `IJK` dimension being less than 4 (except in the case of a two-dimensional calculation). It is also possible that something is fundamentally wrong with the coordinates of the computational domain. Diagnose the problem by checking the `MESH` lines in the input file.

4.3 Support Requests and Bug Tracking

Because FDS development is on-going, problems will inevitably occur with various routines and features. The developers need to know if a certain feature is not working, and reporting problems is encouraged. However, the problem must be clearly identified. The best way to do this is to simplify the input file as much as possible so that the bug can be diagnosed. Also, limit the bug reports to those features that clearly do not work. Physical problems such as fires that do not ignite, flames that do not spread, *etc.*, may be related to the mesh resolution or scenario formulation and need to be investigated first by the user before being reported. If an error message originates from the operating system as opposed to FDS, first investigate some of the more obvious possibilities, such as memory size, disk space, *etc.*

If that does not solve the problem, report the problem with as much information about the error message and circumstances related to the problem. The input file should be simplified as much as possible so that the bug occurs early in the calculation. Attach the simplified input file if necessary, following the instructions provided at the web site. In this way, the developers can quickly run the problem input file and hopefully diagnose the problem.

NOTE: Reports of specific problems, feature requests and enhancements should be posted to the Issue Tracker and not the Discussion Group.

4.4 Known Issues

As a result of collecting feedback from FDS users over roughly a decade, we have identified a number of features in FDS that can be problematic for a variety of reasons. Table 4.1 lists these features that are either under development, or that have been cited a number of times by users who have observed spurious behavior, inconsistent or inaccurate results, fragility, and so on. For those interested in FDS model development, this list is ripe for further research. For those who use FDS for engineering applications, these may be features to avoid until they can be made more reliable and robust.

Table 4.1: Parameters or features known to have problems related to accuracy, numerical stability, robustness, sensitivity, and so on.

Feature	Description	Symptom of Problem	Recommendation
BAROCLINIC	Restores the baroclinic torque term to the momentum equation	Erratic fluid motion, numerical instability in multiple mesh simulations	Reconfigure meshes
CO_PRODUCTION	Algorithm to predict CO production	Inaccuracies found in comparison to experiments	Research usage only
Liquid Fuels	Pyrolysis model of evaporating liquid fuel	Inaccuracies found in comparison to experiments; physical and numerical sensitivity	Research usage only
PRESSURE_CORRECTION	Improve accuracy of pressure solver over multiple meshes	Erratic fluid motion	Do not use if results are unphysical
Solid Fuels	Pyrolysis model of solid fuel	Results in FDS 5.4 and beyond different than previous versions	Read Section 8.3.2

Part II

Writing an FDS Input File

Chapter 5

The Basic Structure of an Input File

5.1   Naming the Job

The operation of FDS is based on a single input text[1] file containing parameters organized into *namelist* [2] groups. The input file provides FDS with all of the necessary information to describe the scenario. The input file is saved with a name such as **job_name.fds**, where **job_name** is any character string that helps to identify the simulation. If this same string is repeated under the `HEAD` namelist group within the input file, then all of the output files associated with the calculation will then have this common name.

There should be no blank spaces in the job name. Instead use the underscore character to represent a space. Using an underscore characters instead of a space also applies to the general practice of naming directories on your system.

Be aware that FDS will simply over-write the output files of a given case if its assigned name is the same. This is convenient when developing an input file because you save on disk space. Just be careful not to overwrite a calculation that you want to keep.

5.2   Namelist Formatting

Parameters are specified within the input file by using *namelist* formatted records. Each namelist record begins with the ampersand character "`&`" followed immediately by the name of the namelist group, then a comma-delimited list of the input parameters, and finally a forward slash "`/`". For example, the line

```
&DUMP NFRAMES=1800, DT_HRR=10., DT_DEVC=10., DT_PROF=30. /
```

sets various values of parameters contained in the `DUMP` namelist group. The meanings of these various parameters will be explained in subsequent chapters. The namelist records can span multiple lines in the input file, but just be sure to end the record with a "`/`" or else the data will not be understood. Do not add anything to a namelist line other than the parameters and values appropriate for that group. Otherwise, FDS will stop immediately upon execution.

Parameters within a namelist record can be separated by either commas, spaces, or line breaks. It is a good idea to use commas or line breaks, and never use tab stops. Some machines do not recognize the spaces or the length of the tab stops. Comments and notes can be written into the file so long as nothing comes before the `&` except a space and nothing comes between the ampersand `&` and the slash `/` except appropriate parameters corresponding to that particular namelist group.

---

[1] ASCII – American Standard Code for Information Interchange

[2] A *namelist* is a Fortran input record.

The parameters in the input file can be integers (`T_END=5400`), real numbers (`CO_YIELD=0.008`), groups of real numbers or integers (`XYZ=6.04,0.28,3.65`) or (`IJK=90,36,38`), character strings:

    CHID='WTC_05_v5'

groups of character strings:

    SURF_IDS='burner','STEEL','BRICK'

or logical parameters:

    POROUS_FLOOR=.FALSE.

A logical parameter is either `.TRUE.` or `.FALSE.` – the periods are a Fortran convention. Character strings that are listed in this User's Manual must be copied exactly as written – the code is case sensitive and underscores *do* matter.

Most of the input parameters are simply real or integer scalars, like `DT=0.02`, but sometimes the inputs are multidimensional arrays. For example, when describing a particular solid surface, you need to express the mass fractions of multiple materials that are to be found in multiple layers. The input array `MATL_MASS_FRACTION(IL,IC)` is intended to convey to FDS the mass fraction of component `IC` of layer `IL`. For example, if the mass fraction of the second material of the third layer is 0.5, then write

    MATL_MASS_FRACTION(3,2)=0.5

To enter more than one mass fraction, use this notation:

    MATL_MASS_FRACTION(1,1:3)=0.5,0.4,0.1

which means that the first three materials of layer 1 have mass fractions of 0.5, 0.4, and 0.1, respectively. The notation `1:3` means array element 1 through 3, inclusive.

> Note that character strings can be enclosed either by apostrophes or quotation marks. Be careful not to create the input file by pasting text from something other than a simple text editor, in which case the punctuation marks may not transfer properly into the text file.

> Note that depending on compiler and operating system, some text file encodings may not work on all systems. If file reading errors occur and no typographical errors can be found in the input file, try saving the input file using a different encoding. It does not appear that current Fortran compilers support the UTF-8 encoding standard for reading Namelist inputs.

5.3   Input File Structure

In general, the namelist records can be entered in any order in the input file, but it is a good idea to organize them in some systematic way. Typically, general information is listed near the top of the input file, and detailed information, like obstructions, devices, and so on, are listed below. FDS scans the entire input file each time it processes a particular namelist group. With some text editors, it has been noticed that the last line of the file is often not read by FDS because of the presence of an "end of file" character. To ensure that FDS reads the entire input file, add

`&TAIL /`

as the last line at the end of the input file. This completes the file from `&HEAD` to `&TAIL`. FDS does not even look for this last line. It just forces the "end of file" character past relevant input.

Another general rule of thumb when writing input files is to only add to the file parameters that are to change from their default value. That way, you can more easily distinguish between what you want and what

FDS wants. Add comments liberally to the file, so long as these comments do not fall within the namelist records.

The general structure of an input file is shown below, with many lines of the original validation input file[3] removed for clarity.

```
&HEAD CHID='WTC_05_v5', TITLE='WTC Phase 1, Test 5, FDS version 5' /
&MESH IJK=90,36,38, XB=-1.0,8.0,-1.8,1.8,0.0,3.82 /
&TIME T_END=5400. /
&MISC SURF_DEFAULT='MARINITE BOARD', TMPA=20., POROUS_FLOOR=.FALSE. /
&DUMP NFRAMES=1800, DT_HRR=10., DT_DEVC=10., DT_PROF=30. /

&REAC ID         = 'HEPTANE TO CO2'
      FYI        = 'Heptane, C_7 H_16'
      C          = 7.
      H          = 16.
      CO_YIELD   = 0.008 /
      SOOT_YIELD = 0.015 /

&OBST XB= 3.5, 4.5,-1.0, 1.0, 0.0, 0.0, SURF_ID='STEEL FLANGE' /  Fire Pan
...
&SURF ID        = 'STEEL FLANGE'
      COLOR     = 'BLACK'
      MATL_ID   = 'STEEL'
      BACKING   = 'EXPOSED'
      THICKNESS = 0.0063 /
...
&VENT MB='XMIN',SURF_ID='OPEN' /
...
&SLCF PBY=0.0, QUANTITY='TEMPERATURE', VECTOR=.TRUE. /
...
&BNDF QUANTITY='GAUGE HEAT FLUX' /
...
&DEVC XYZ=6.04,0.28,3.65, QUANTITY='oxygen', ID='EO2_FDS' /
...
&TAIL / End of file.
```

It is strongly recommended that when looking at a new scenario, first select a pre-written input file that resembles the case, make the necessary changes, then run the case at fairly low resolution to determine if the geometry is set up correctly. It is best to start off with a relatively simple file that captures the main features of the problem without getting tied down with too much detail that might mask a fundamental flaw in the calculation. Initial calculations ought to be meshed coarsely so that the run times are less than an hour and corrections can easily be made without wasting too much time. As you learn how to write input files, you will continually run and re-run your case as you add in complexity.

Table 5.1 provides a quick reference to all the namelist parameters and where you can find the reference to where it is introduced in the document and the table containing all of the keywords for each group.

---

[3]The actual input file, WTC_05_v5.fds, is part of the FDS Validation Suite

Table 5.1: Namelist Group Reference Table

Group Name	Namelist Group Description	Reference Section	Parameter Table
BNDF	Boundary File Output	14.2.4	15.1
CTRL	Control Function Parameters	13.5	15.3
DEVC	Device Parameters	13.1	15.4
DUMP	Output Parameters	14.1	15.5
HEAD	Input File Header	6.1	15.6
HOLE	Obstruction Cutout	7.3	15.7
INIT	Initial Condition	6.5	15.8
ISOF	Isosurface File Output	14.2.5	15.9
MATL	Material Property	8.2	15.10
MESH	Mesh Parameters	6.3	15.11
MISC	Miscellaneous	6.4	15.12
MULT	Multiplier Parameters	7.2.2	15.13
OBST	Obstruction	7.2	15.14
PART	Lagrangian Particle	12	15.15
PROF	Profile Output	14.2.2	15.16
PROP	Device Property	13.3	15.17
RADI	Radiation	11.3	15.18
RAMP	Ramp Profile	10	15.19
REAC	Reactions	11.1	15.20
SLCF	Slice File Output	14.2.3	15.21
SPEC	Species Parameters	11.2	15.22
SURF	Surface Properties	7.1	15.23
TIME	Simulation Time	6.2	15.25
TRNX	Mesh Stretching	6.3.5	15.26
VENT	Vent Parameters	7.4	15.27
ZONE	Pressure Zone Parameters	9.6	15.28

Chapter 6

Setting the Bounds of Time and Space

6.1 Naming the Job: The `HEAD` Namelist Group (Table 15.6)

The first thing to do when setting up an input file is to give the job a name. The name of the job is important because often a project involves numerous simulations in which case the names of the individual simulations can help organize the effort. The namelist group `HEAD` contains two parameters, as in this example:

```
&HEAD CHID='WTC_05_v5', TITLE='WTC Phase 1, Test 5, FDS version 5' /
```

`CHID` is a string of 30 characters or less used to tag the output files. If, for example, `CHID='WTC_05_v5'`, it is convenient to name the input data file `WTC_05_v5.fds` so that the input file can be associated with the output files. No periods or spaces are allowed in `CHID` because the output files are tagged with suffixes that are meaningful to certain computer operating systems.

`TITLE` is a string of 60 characters or less that describes the simulation. It is simply descriptive text that is passed to various output files.

6.2 Simulation Time: The `TIME` Namelist Group (Table 15.25)

`TIME` is the name of a group of parameters time define the time duration of the simulation and the initial time step used to advance the solution of the discretized equations.

6.2.1 Basics

Usually, only the duration of the simulation is required on this line, via the parameter `T_END`. The default is 1 s. Note: the older `TWFIN` will still work but it has been deprecated, it is recommended that `T_END` be used now instead.

For example, the following line will instruct FDS to run the simulation for 5400 seconds.

```
&TIME T_END=5400. /
```

If `T_END` is set to zero, only the set-up work is performed, allowing you to quickly check the geometry in Smokeview.

If you want the time line to start at a number other than zero, you can use the parameter `T_BEGIN` to specify the time written to file for the first time step. This would be useful for matching time lines of experimental data or video recordings.

Time-based RAMPs are evaluated using the actual time if the RAMP activation time is the same as T_BEGIN; otherwise, they are evaluated using the time from when the RAMP activates. Therefore, if you are setting T_BEGIN in order to test a time-based CTRL or DEVC that is ultimately linked to a RAMP, then you should set T_BEGIN to be slightly less than the time the RAMP will activate. For example if you are testing a VENT that is to open at 10 s whose SURF_ID uses a RAMP, T_BEGIN should be set slightly less than 10 s.

6.2.2 Special Topic: Controlling the Time Step

The initial time step size can be specified with DT. This parameter is normally set automatically by dividing the size of a mesh cell by the characteristic velocity of the flow. During the calculation, the time step is adjusted so that the CFL (Courant, Friedrichs, Lewy) condition is satisfied. The default value of DT is $5(\delta x\,\delta y\,\delta z)^{\frac{1}{3}}/\sqrt{gH}$ s, where δx, δy, and δz are the dimensions of the smallest mesh cell, H is the height of the computational domain, and g is the acceleration of gravity. Note that by default the time step is never allowed to increase above its initial value. To allow this to happen, set RESTRICT_TIME_STEP=.FALSE.

If something sudden is to happen right at the start of a simulation, like a sprinkler activation, it is a good idea to set the initial time step to avoid a numerical instability caused by too large a time step. Experiment with different values of DT by monitoring the initial time step sizes recorded in the output file **job_name.out**.

One additional parameter in the TIME group is SYNCHRONIZE, a logical flag (.TRUE. or .FALSE.) indicating that in a multi-mesh computation the time step for each mesh should be the same, thus ensuring that each mesh is processed each iteration. More details can be found in Section 6.3.3. The default value of SYNCHRONIZE is .TRUE.

Finally, if you want to prevent FDS from automatically changing the time step, set
LOCK_TIME_STEP=.TRUE.
on the TIME line, in which case the specified time step, DT, will not be adjusted. This parameter is intended for diagnostic purposes only, for example, timing program execution. It can lead to numerical instabilities if the initial time step is set too high.

6.2.3 Special Topic: Steady-State Applications

Occasionally, there are applications in which only the steady-state solution (in a time-averaged sense) is desired. However, the time necessary to heat the walls to steady-state can make the cost of the calculation prohibitive. In these situations, if you specify a TIME_SHRINK_FACTOR of, say, 10, the specific heats of the various materials is reduced by a factor of 10, speeding up the heating of these materials roughly by 10. An example of an application where this parameter is handy is a validation experiment where a steady heat source warms up a compartment to a nearly equilibrium state at which point time-averaged flow quantities are measured.

6.3 Computational Meshes: The MESH Namelist Group (Table 15.11)

All FDS calculations must be performed within a domain that is made up of rectilinear volumes called *meshes*. Each mesh is divided into rectangular *cells*, the number of which depends on the desired resolution of the flow dynamics. MESH is the namelist group that defines the computational domain.

6.3.1 Basics

A mesh is a single right parallelepiped, *i.e.* a box. The coordinate system within a mesh conforms to the right hand rule. The origin point of a mesh is defined by the first, third and fifth values of the real number sextuplet, XB, and the opposite corner is defined by the second, fourth and sixth values. For example,

```
&MESH IJK=10,20,30, XB=0.0,1.0,0.0,2.0,0.0,3.0 /
```

defines a mesh that spans the volume starting at the origin and extending 1 m in the positive x direction, 2 m in the positive y direction, and 3 m in the positive z direction. The mesh is subdivided into uniform cells via the parameter IJK. In this example, the mesh is divided into 10 cm cubes. If it is desired that the mesh cells in a particular direction not be uniform in size, then the namelist groups TRNX, TRNY and/or TRNZ may be used to alter the uniformity of the mesh (See Section 6.3.5).

Any obstructions or vents that extend beyond the boundary of the mesh are cut off at the boundary. There is no penalty for defining objects outside of the mesh, and these objects will not appear in Smokeview.

> Note that it is best if the mesh cells resemble cubes, that is, the length, width and height of the cells ought to be roughly the same.

Because an important part of the calculation uses a Poisson solver based on Fast Fourier Transforms (FFTs) in the y and z directions, the second and third dimensions of the mesh should each be of the form $2^l \, 3^m \, 5^n$, where l, m and n are integers. For example, $64 = 2^6$, $72 = 2^3 3^2$ and $108 = 2^2 3^3$ are good mesh cell divisions, but 37, 99 and 109 are not. The first number of mesh cell divisions (the I in IJK) does not use FFTs and need not be given as a product of small numbers. However, you should experiment with different values of divisions to ensure that those that are ultimately used do not unduly slow down the calculation.

Here is a list of numbers between 1 and 1024 that can be factored down to 2's, 3's and 5's:

```
  2    3    4    5    6    8    9   10   12   15   16   18   20   24   25
 27   30   32   36   40   45   48   50   54   60   64   72   75   80   81
 90   96  100  108  120  125  128  135  144  150  160  162  180  192  200
216  225  240  243  250  256  270  288  300  320  324  360  375  384  400
405  432  450  480  486  500  512  540  576  600  625  640  648  675  720
729  750  768  800  810  864  900  960  972 1000 1024
```

6.3.2 Two-Dimensional and Axially-Symmetric Calculations

The governing equations solved in FDS are written in terms of a three dimensional Cartesian coordinate system. However, a two dimensional Cartesian or two dimensional cylindrical (axially-symmetric) calculation can be performed by setting the J in the IJK triplet to 1 on the MESH line. For axial symmetry, add CYLINDRICAL=.TRUE. to the MESH line, and the coordinate x is then interpreted as the radial coordinate r. No boundary conditions should be set at the planes $y = $ YMIN=XB(3) or $y = $ YMAX=XB(4), nor at $r = $ XMIN=XB(1) in an axially-symmetric calculation in which $r = $ XB(1)=0. For better visualizations, the difference between XB(4) and XB(3) should be small so that the Smokeview rendering appears to be in 2-D. An example of an axially-symmetric helium plume (**helium_2d**) is given in Section 6.4.5.

6.3.3 Multiple Meshes and Parallel Processing
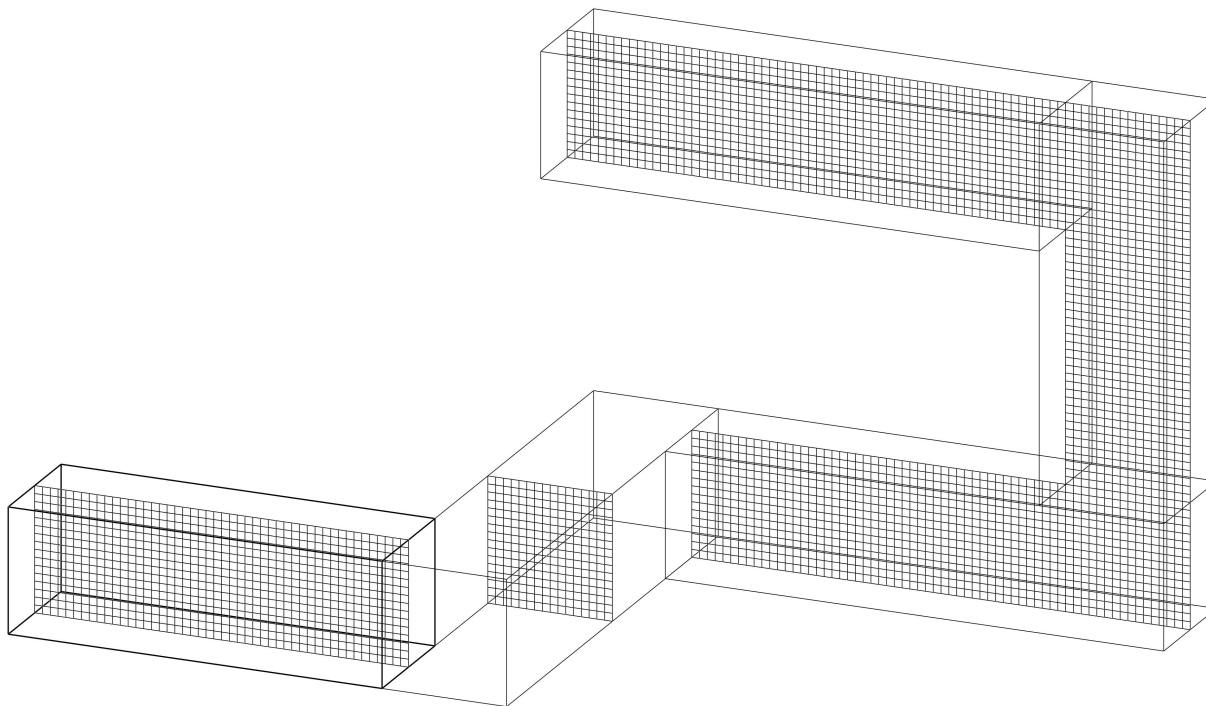
Figure 6.1: An example of a multiple-mesh geometry.

The term "multiple meshes" means that the computational domain consists of more than one computational mesh, usually connected although this is not required. If more than one mesh is used, there should be a MESH line for each. The order in which these lines are entered in the input file matters. In general, the meshes should be entered from finest to coarsest. FDS assumes that a mesh listed first in the input file has precedence over a mesh listed second if the two meshes overlap. Meshes can overlap, abut, or not touch at all. In the last case, essentially two separate calculations are performed with no communication at all between them. Obstructions and vents are entered in terms of the overall coordinate system and need not apply to any one particular mesh. Each mesh checks the coordinates of all the geometric entities and decides whether or not they are to be included.

To run FDS in parallel using MPI (Message Passing Interface), you **must** break up the computational domain into multiple meshes so that the workload can be divided among the available processors. In general, it is better to run multiple mesh cases with the parallel version of FDS if you have the computers available, but be aware that two computers will not necessarily finish the job in half the time as one. For the parallel version to work well, there has to be a comparable number of cells in each mesh, or otherwise most of the computers will sit idle waiting for the one with the largest mesh to finish processing each time step. You can use multiple meshes even when running the serial version of FDS, in which case one CPU will serially process each mesh, one by one. Why do this? For one, if you set
SYNCHRONIZE=.FALSE.
on the TIME line, then in each mesh, the governing equations will be solved with a time step based on the flow speed within that particular mesh. Because each mesh can have different time steps, this technique can save CPU time by requiring relatively coarse meshes to be updated only when necessary. Coarse meshes

are best used in regions where temporal and spatial gradients of key quantities are small or unimportant. Be aware, however, that unsynchronized time steps are more likely to lead to numerical instabilities.

By default, the time steps in each mesh are synchronized. With this setting, all meshes are active each iteration. For a single-processor, multiple mesh calculation, this strategy reduces and may even eliminate any benefit seen by using multiple meshes. However, in a parallel calculation, if a particular mesh is inactive during an iteration because it is not ready to be updated, then the processor assigned to that mesh is also inactive. Forcing the mesh to be updated with a smaller than ideal time step does not cost anything since that processor would have been idle anyway. The benefit is that there is a tighter connection between meshes. It is also possible to synchronize the time step in only a select set of meshes. To do this, add `SYNCHRONIZE=.TRUE.` to the appropriate `MESH` lines and then add `SYNCHRONIZE=.FALSE.` to the `TIME` line.

Usually in a multi-mesh calculation, each mesh is assigned its own process, and each process its own processor. However, it is possible to assign more than one mesh to a single process, and it is possible to assign more than one process to a single processor. Consider a case that involves six meshes:

```
&MESH ID='mesh1', IJK=..., XB=..., MPI_PROCESS=0 /
&MESH ID='mesh2', IJK=..., XB=..., MPI_PROCESS=1 /
&MESH ID='mesh3', IJK=..., XB=..., MPI_PROCESS=1 /
&MESH ID='mesh4', IJK=..., XB=..., MPI_PROCESS=2 /
&MESH ID='mesh5', IJK=..., XB=..., MPI_PROCESS=3 /
&MESH ID='mesh6', IJK=..., XB=..., MPI_PROCESS=3 /
```

The parameter `MPI_PROCESS` instructs FDS to assign that particular mesh to the given process. In this case, only four processes are to be started, numbered 0 through 3. Note that the processes need to be invoked in ascending order, starting with 0. Why would you do this? Suppose you only have four processors available for this job. By starting only four processes instead of six, you can save time because 'mesh2' and 'mesh3' can communicate directly with each other without having to transmit data using MPI calls over the network. Same goes for 'mesh5' and 'mesh6'. In essence, it is as if these mesh pairs are neighbors and need not send mail to each other via the postal system. The letters can just be walked next door.

6.3.4 Mesh Alignment

Whether the calculation is to be run on a single processor, or on multiple processors, the rules of prescribing multiple meshes are similar, with some issues to keep in mind. The most important rule of mesh alignment is that abutting cells ought to have the same cross sectional area, or integral ratios, as shown in Fig. 6.2. The requirement of integral mesh alignment is new starting with FDS version 5.1. It is a more restrictive requirement than in previous versions because it was becoming too difficult to maintain complete flexibility in alignment while trying to improve the accuracy of the methodology. The following rules of thumb should also be followed when setting up a multiple mesh calculation:

- Avoid putting mesh boundaries where critical action is expected, especially fire. Sometimes fire spread from mesh to mesh cannot be avoided, but if at all possible try to keep mesh interfaces relatively free of complicated phenomena since the exchange of information across mesh boundaries is not yet as accurate as cell to cell exchanges within one mesh.

- In general, there is little advantage to overlapping meshes because information is only exchanged at exterior boundaries. This means that a mesh that is completely embedded within another receives information at its exterior boundary, but the larger mesh receives no information from the mesh embedded within. Essentially, the larger, usually coarser, mesh is doing its own simulation of the scenario and is not affected by the smaller, usually finer, mesh embedded within it. Details within the fine mesh,
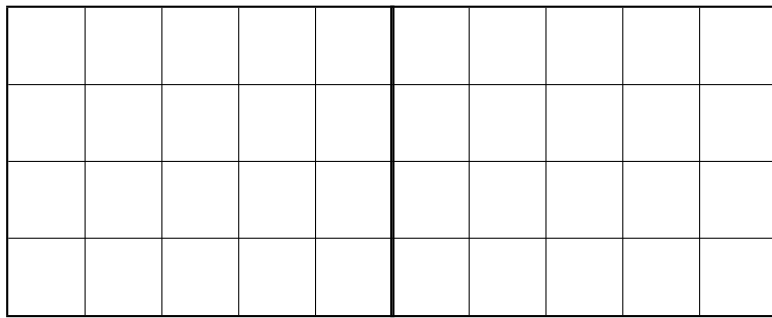
This is the ideal kind of mesh to mesh alignment.
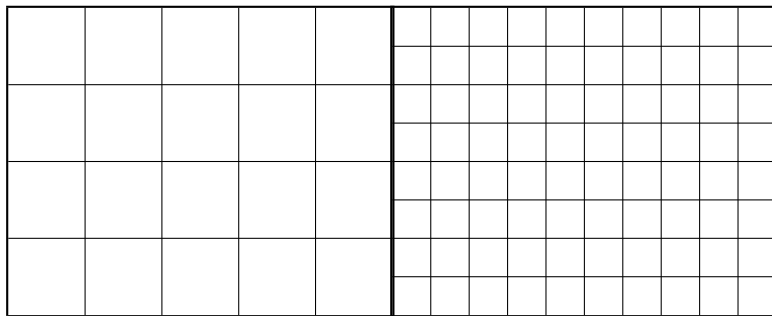
This is allowed so long as there are an integral number of fine cells abutting each coarse cell.
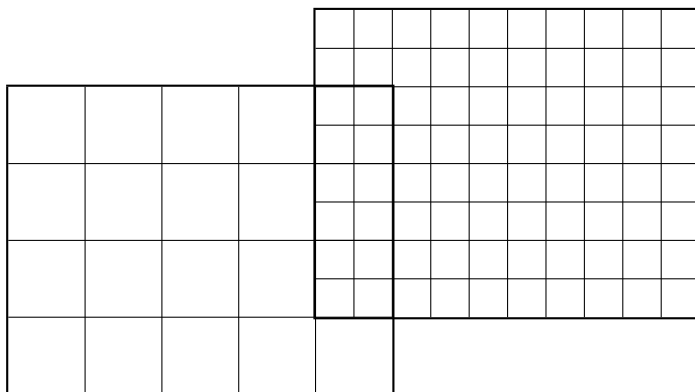
This is allowed, but of questionable value.
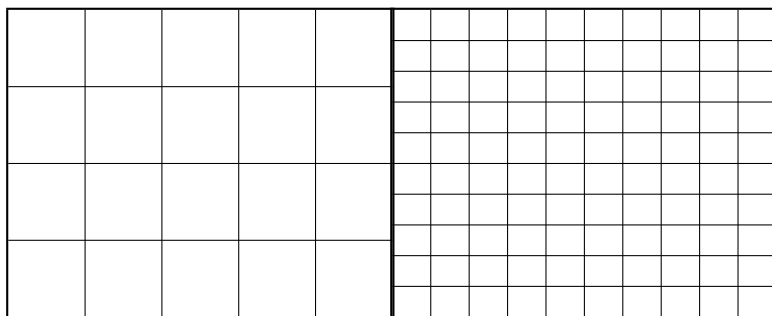
This is no longer allowed in FDS 5.1 and higher.

Figure 6.2: Rules governing the alignment of meshes.

especially related to fire growth and spread, may not be picked up by the coarse mesh. In such cases, it is preferable to isolate the detailed fire behavior within one mesh, and position coarser meshes at the exterior boundary of the fine mesh. Then the fine and coarse meshes mutually exchange information.

- Be careful when using the shortcut convention of declaring an entire face of the domain to be an OPEN vent. Every mesh takes on this attribute. See Section 7.4 for more details.

- If a planar obstruction is close to where two meshes abut, make sure that each mesh "sees" the obstruction. If the obstruction is even a millimeter outside of one of the meshes, that mesh does not account for it, in which case information is not transferred properly between meshes.

Accuracy of the Parallel Calculation

Experiment with different mesh configurations using relatively coarse mesh cells to ensure that information is being transferred properly from mesh to mesh. There are two issues of concern. First, does it appear that the flow is being badly affected by the mesh boundary? If so, try to move the mesh boundaries away from areas of activity. Second, is there too much of a jump in cell size from one mesh to another? If so, consider whether the loss of information moving from a fine to a coarse mesh is tolerable.

Efficiency of the Parallel Calculation

When running a case with multiple meshes in parallel, the efficiency of the calculation can be checked as follows: (1) Set SYNCHRONIZE=.TRUE. on the TIME line, (2) Let the program run several hundred time steps, (3) Calculate the difference in wall clock time between two 100 iteration print outs in the file **CHID.out** (see Section 19.1). Divide the time difference by 100. This is the average elapsed wall clock time per time step, (4) Look at the CPU/step for each mesh. The largest value should be less than, but close to, the average elapsed wall clock time. The efficiency of the parallel calculation is the maximum CPU/step divided by the average wall clock time per step. If this number is between 90 % and 100 %, the parallel code is working well.

6.3.5 Mesh Stretching: The TRNX, TRNY and/or TRNZ Namelist Groups (Table 15.26)

By default the mesh cells that fill the computational domain are uniform in size. However, it is possible to specify that the cells be non-uniform in one or two of the three coordinate directions. For a given coordinate direction, *x*, *y* or *z*, a function can be prescribed that transforms the uniformly-spaced mesh to a non-uniformly spaced mesh. **Be careful with mesh transformations!** If you shrink cells in one region you must stretch cells somewhere else. When one or two coordinate directions are transformed, the aspect ratio of the mesh cells in the 3D mesh will vary. To be on the safe side, transformations that alter the aspect ratio of cells beyond 2 or 3 should be avoided. Keep in mind that the large eddy simulation technique is based on the assumption that the numerical mesh should be fine enough to allow the formation of eddies that are responsible for the mixing. In general, eddy formation is limited by the largest dimension of a mesh cell, thus shrinking the mesh resolution in one or two directions may not necessarily lead to a better simulation if the third dimension is large.

Transformations, in general, reduce the efficiency of the computation, with two coordinate transformations impairing efficiency more than a transformation in one coordinate direction. Experiment with different meshing strategies to see how much of a penalty you will pay.

Here is an example of how to do a mesh transformation. Suppose your mesh is defined
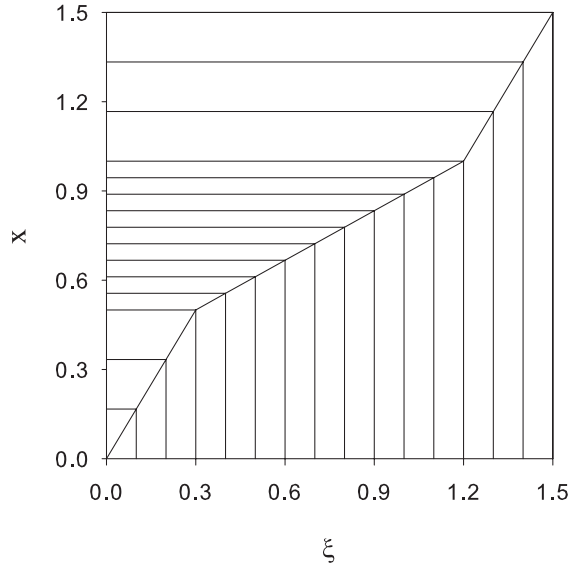
Figure 6.3: Piecewise-Linear Mesh Transformation.
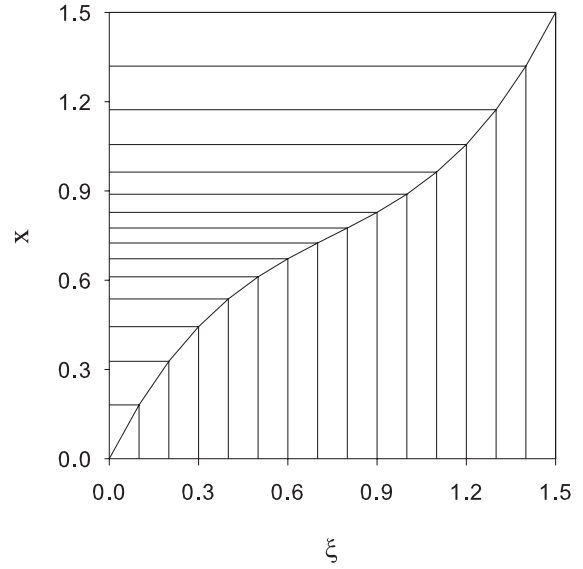
Figure 6.4: Polynomial Mesh Transformation.

```
&MESH IJK=15,10,20, XB=0.0,1.5,1.2,2.2,3.2,5.2 /
```

and you want to alter the uniform spacing in the x direction. First, refer to the figures above. You need to define a function $x = f(\xi)$ that maps the uniformly-spaced *Computational Coordinate* (CC) $0 \leq \xi \leq 1.5$ to the *Physical Coordinate* (PC) $0 \leq x \leq 1.5$. The function has three mandatory constraints: it must be monotonic (always increasing), it must map $\xi = 0$ to $x = 0$, and it must map $\xi = 1.5$ to $x = 1.5$. The default transformation function is $f(\xi) = \xi$ for a uniform mesh, but you need not do anything in this case.

Two types of transformation functions are allowed. The first, and simplest, is a piecewise-linear function. Figure 6.3 gives an example of a piecewise-linear transformation. The graph indicates how 15 uniformly spaced mesh cells along the horizontal axis are transformed into 15 non-uniformly spaced cells along the vertical axis. In this case, the function is made up of straight line segments connecting points (CC,PC), in increasing order, as specified by the following lines in the input file:

```
&TRNX CC=0.30, PC=0.50, MESH_NUMBER=2 /
&TRNX CC=1.20, PC=1.00, MESH_NUMBER=2 /
```

The parameter CC refers to the Computational Coordinate, ξ, located on the horizontal axis; PC is the Physical Coordinate, x, located on the vertical axis. The slopes of the line segments in the plot indicate whether the mesh is being stretched (slopes greater than 1) or shrunk (slopes less than 1). The tricky part about this process is that you usually have a desired shrinking/stretching strategy for the Physical Coordinate on the vertical axis, and must work backwards to determine what the corresponding points should be for the Computational Coordinate on the horizontal axis. Note that the above transformation is applied to the second mesh in a multiple mesh job.

The second type of transformation is a polynomial function whose constraints are of the form

$$\frac{d^n f(\text{CC})}{d\xi^n} = \text{PC}$$

34

Figure 6.4 gives an example of a polynomial transformation, for which the parameters are specified (assuming that this is the third mesh):

```
&TRNX IDERIV=0, CC=0.75, PC=0.75, MESH_NUMBER=3 /
&TRNX IDERIV=1, CC=0.75, PC=0.50, MESH_NUMBER=3 /
```

which correspond to the constraints $f(0.75) = 0.75$ and $\frac{df}{d\xi}(0.75) = 0.5$, or, in words, the function maps 0.75 into 0.75 and the slope of the function at $\xi = 0.75$ is 0.5. The transform function must also pass through the points (0,0) and (1.5,1.5), meaning that FDS must compute the coefficients for the cubic polynomial $f(\xi) = c_0 + c_1 \xi + c_2 \xi^2 + c_3 \xi^3$. More constraints on the function lead to higher order polynomial functions, so be careful about too many constraints which could lead to non-monotonic functions. The monotonicity of the function is checked by the program and an error message is produced if it is not monotonic.

Do not specify either linear transformation points or `IDERIV=0` points at coordinate values corresponding to the mesh boundaries.

6.3.6 Choosing Optimum Mesh Dimensions

A common question asked by new FDS users is, "What size mesh should I use?" The answer is not easy because it depends considerably on what you are trying to accomplish. In general, you should build an FDS input file using a relatively coarse mesh, and then gradually refine the mesh until you do not see appreciable differences in your results. Formally, this is referred to as a mesh sensitivity study.

For simulations involving buoyant plumes, a measure of how well the flow field is resolved is given by the non-dimensional expression $D^*/\delta x$, where D^* is a characteristic fire diameter

$$D^* = \left(\frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{g}} \right)^{\frac{2}{5}} \tag{6.1}$$

and δx is the nominal size of a mesh cell[1]. The quantity $D^*/\delta x$ can be thought of as the number of computational cells spanning the characteristic (not necessarily the physical) diameter of the fire. The more cells spanning the fire, the better the resolution of the calculation. It is better to assess the quality of the mesh in terms of this non-dimensional parameter, rather than an absolute mesh cell size. For example, a cell size of 10 cm may be "adequate," in some sense, for evaluating the spread of smoke and heat through a building from a sizable fire, but may not be appropriate to study a very small, smoldering source[2].

---

[1]The characteristic fire diameter is related to the characteristic fire size via the relation $Q^* = (D^*/D)^{5/2}$, where D is the physical diameter of the fire.

[2]For the validation study sponsored by the U.S. Nuclear Regulatory Commission [4], the $D^*/\delta x$ values ranged from 4 to 16.

6.4   Miscellaneous Parameters: The `MISC` Namelist Group (Table 15.12)

`MISC` is the namelist group of global miscellaneous input parameters. It contains parameters that do not logically fit into any other category.

6.4.1   Basics

Only one `MISC` line should be entered in the data file. For example, the input line

```
&MISC SURF_DEFAULT='CONCRETE',TMPA=25. /
```

establishes that all bounding surfaces are to be made of `CONCRETE` unless otherwise specified, and that the ambient temperature is 25 °C.

The `MISC` parameters vary in scope and degree of importance. Here is a partial list of `MISC`ellaneous parameters. Others are described where necessary throughout this guide.

`DNS` A logical parameter that, if `.TRUE.`, directs FDS to perform a Direct Numerical Simulation, as opposed to the default Large Eddy Simulation (LES). This feature is appropriate only for simulations that use mesh cells that are on the order of a millimeter or less in size, or for diagnostic purposes.

`GVEC` The 3 components of gravity, in m/s^2. The default is `GVEC=0,0,-9.81`.

`HUMIDITY` Relative humidity, in units of %. This need only be specified if there is a source of water in the simulation other than the fire itself. Otherwise, water vapor is not explicitly tracked. Default 40 %.

`ISOTHERMAL` A logical parameter that indicates that the calculation does not involve any changes in temperature or radiation heat transfer, thus reducing the number of equations that must be solved, and simplifying those that are. Automatically sets `RADIATION` to `.FALSE.`

`NOISE` FDS initializes the flow field with a very small amount of "noise" to prevent the development of a perfectly symmetric flow when the boundary and initial conditions are perfectly symmetric. To turn this off, set `NOISE=.FALSE.`

`P_INF` Background pressure (at the ground) in Pa. The default is 101325 Pa.

`RADIATION` A logical parameter indicating whether radiation transport ought to be calculated. The default is `.TRUE.`

`SUPPRESSION` A logical parameter indicating whether FDS should include gas phase flame extinction. The default is `.TRUE.`

`SURF_DEFAULT` The `SURF` line that is to be applied to all boundaries, unless otherwise specified. The default is `'INERT'`, a non-reacting solid boundary whose temperature is fixed at `TMPA`. You do not need to define `'INERT'` via a `SURF` line.

`TMPA` Ambient temperature, the temperature of everything at the start of the simulation. The default is 20 °C.

`U0, V0, W0` Initial values of the gas velocity in each of the coordinate directions. Normally, these are all 0 m/s, but there are a few applications where it is convenient to start the flow immediately, like in an outdoor simulation involving wind.

6.4.2 Special Topic: Stopping and Restarting Calculations

An important `MISC` parameter is called `RESTART`. Normally, a simulation consists of a sequence of events starting from ambient conditions. However, there are occasions when you might want to stop a calculation, make a few limited adjustments, and then restart the calculation from that point in time. To do this, first bring the calculation to a halt gracefully by creating a file called **CHID.stop** in the directory where the output files are located. Remember that FDS is case-sensitive. The file name must be exactly the same as the `CHID` and 'stop' should be lower case. FDS checks for the existence of this file at each time step, and if it finds it, gracefully shuts down the calculation after first creating a final Plot3D file and a file (or files in the case of a multiple mesh job) called **CHID.restart** (or **CHID_nn.restart**). To restart a job, the file(s) **CHID.restart** should exist in the working directory, and the phrase `RESTART=.TRUE.` needs to be added to the `MISC` line of the input data file. For example, suppose that the job whose `CHID` is "plume" is halted by creating a dummy file called **plume.stop** in the directory where all the output files are being created. To restart this job from where it left off, add `RESTART=.TRUE.` to the `MISC` line of the input file **plume.fds**, or whatever you have chosen to name the input file. The existence of a restart file with the same `CHID` as the original job tells FDS to continue saving the new data in the same files as the old. If `RESTART_CHID` is also specified on the `MISC` line, then FDS will look for old output files tagged with this string instead of using the specified `CHID` on the `HEAD` line. In this case, the new output files will be tagged with `CHID`, and the old output files will not be altered.

When running the restarted job, the diagnostic output of the restarted job is appended to the file **CHID.out** that was created by the original job. All of the other output files from the original run are appended as well.

There may be times when you want to save restart files periodically during a run as insurance against power outages or system crashes. If this is the case, at the start of the original run set `DT_RESTART=50.` on the `DUMP` line to save restart files every 50 s, for example. The default for `DT_RESTART` is 1000000, meaning no restart files are created unless you gracefully stop a job by creating a dummy file called **CHID.stop**.

It is also possible to use the new control function feature (see Section 13.5) to stop a calculation or dump a restart file when the computation reaches some measurable condition such as a first sprinkler activation.

Between job stops and restarts, major changes cannot be made in the calculation like adding or removing vents and obstructions. The changes are limited to those parameters that do not instantly alter the existing flow field. Since the restart capability has been used infrequently by the developers, it should be considered a fragile construct. Examine the output to ensure that no sudden or unexpected events occur during the stop and restart.

6.4.3 Special Topic: Defying Gravity

Most users of FDS assume that the acceleration of gravity points in the negative z direction, or more simply, downward. However, to change the direction of gravity to model a sloping roof or tunnel, for example, specify the gravity vector on the `MISC` line with a triplet of numbers of the form `GVEC=0.,0.,-9.81`, with units of m/s^2. This is the default, but it can be changed to be any direction.

There are a few special applications where you might want to vary the gravity vector as a function of time or as a function of the first spatial coordinate, x. For example, on board the Space Shuttle or International Space Station, small motions can cause temporal changes in the normally zero level of gravity, an effect known as "g-jitter." More commonly, in tunnel fire simulations, it is sometimes convenient to change the direction of gravity to mimic the change in slope. The slope of the tunnel might change as you travel through it; thus, you can tell FDS where to redirect gravity. For either a spatially or temporally varying direction and/or magnitude of gravity, do the following. First, on the `MISC` line, set the three components of gravity, `GVEC`, to some "base" state like `GVEC=1.,1.,1.`, which gives you the flexibility to vary all three components. Next, designate "ramps" for the individual components, `RAMP_GX`, `RAMP_GY`, and `RAMP_GZ`,

all of which are specified on the MISC line. There is more discussion of RAMPs in Section 10, but for now you can use the following as a simple template to follow:

```
&MISC GVEC=1.,0.,1., RAMP_GX='x-ramp', RAMP_GZ='z-ramp' /

&RAMP ID='x-ramp', X=  0., F=0.0 /
&RAMP ID='x-ramp', X= 50., F=0.0 /
&RAMP ID='x-ramp', X= 51., F=-0.49 /
&RAMP ID='x-ramp', X=100., F=-0.49 /

&RAMP ID='z-ramp', X=  0., F=-9.81 /
&RAMP ID='z-ramp', X= 50., F=-9.81 /
&RAMP ID='z-ramp', X= 51., F=-9.80 /
&RAMP ID='z-ramp', X=100., F=-9.80 /
```

Note that both the x and z components of gravity are functions of x. FDS has been programmed to only allow variation in the x coordinate. Note also that F is just a multiplier of the "base" gravity vector components, given by GVEC. This is why using the number 1 is convenient – it allows you to specify the gravity components on the RAMP lines directly. The effect of these lines is to model the first 50 m of a tunnel without a slope, but the second 50 m with a 5 % slope upwards. Note that the angle from vertical of the gravity vector due to a 5 % slope is $\tan^{-1} 0.05 = 2.86°$ and that 0.49 and 9.80 are equal to the magnitude of the gravity vector, 9.81 m/s^2, multiplied by the sine and cosine of 2.86°, respectively. To check your math, the sum of the squares of the gravity components ought to equal 9.81. Notice in this case that the y direction has been left out because there is no y variation in the gravity vector.

To vary the direction and/or magnitude of gravity in time, follow the same procedure but replace the X in the RAMP lines with a T.

6.4.4 Special Topic: Improving the Pressure Solver

FDS uses a low-Mach number formulation of the Navier-Stokes equations. One of the consequences of this is that the speed of sound is assumed infinite, and that the pressure throughout the computational domain is affected, instantaneously, by local changes in the flow field. A simple example of this is when air is pushed through a tunnel. If the tunnel has forced flow at one end and an opening at the other, the volume flow at the opening is the same as that which is forced at the other end. Without any heat addition, the air is assumed incompressible. Information is passed through the tunnel instantaneously in the model via a solution of a linear system of equations for the pressure. For a single mesh, the solution of this Poisson equation for the pressure is very accurate. However, for multiple meshes, there is potentially a delay in information passing throughout the domain because the Poisson equation is solved on each individual mesh, without any influence from the larger computational domain. The details of the numerics can be found in the FDS Technical Reference Guide.

A new feature has been added in FDS 5 to improve the accuracy of the multi-mesh pressure solver. Briefly, a correction is made to the local solutions of the Poisson equation by way of a global solution for an "average" pressure in each mesh. This can be thought of as the pressure that one would obtain from a zone or lumped parameter model where each compartment in a building has its own bulk pressure obtained via mass balance estimates at compartment boundaries. Currently, this pressure correction is still an option because it requires additional testing and it requires additional CPU time. To invoke it, add

```
PRESSURE_CORRECTION=.TRUE.
```

to the MISC line. Run your case with and without the option to determine how much additional CPU time is required, and also how much of an improvement in accuracy it yields. This can be done in two ways. First, examine vector slice files of various quantities at the mesh boundaries to see if there are noticeable changes

in the flow field due to the boundary. Second, add

`CHECK_VOLUME_FLOW=.TRUE.`

to the `DUMP` line, just for debugging purposes. This will prompt FDS to compute the volume flow at each mesh boundary to determine if the pressure correction scheme is working properly. If error messages appear on the screen or in the standard error file, post the case to the Issue Tracker.

If `PRESSURE_CORRECTION=.TRUE.`, the meshes cannot overlap. Also, if two adjacent meshes are of different resolution, any obstruction crossing the mesh interface must conform to the more coarse of the two. Otherwise, volume cannot be conserved.

6.4.5 Special Topic: Restoring the Baroclinic Vorticity

There is an approximation made when solving for the pressure where it is assumed that

$$\nabla \cdot \frac{1}{\rho} \nabla \tilde{p} = \frac{1}{\rho_\infty} \nabla^2 \tilde{p}. \tag{6.2}$$

The consequence of this approximation is that the vorticity generated due to the non-alignment of the density and pressure gradients, or the baroclinic torque, is neglected. For most large scale applications, the assumption is justified by the fact that the vorticity generated by buoyancy is the dominant source of vorticity. By neglecting the baroclinic torque the solution of the elliptic partial differential equation obtained by taking the divergence of the momentum equation is greatly simplified. However, an option exists in the code to restore the baroclinic torque by decomposing the relevant term in the pressure equation as follows,

$$\nabla \cdot \frac{1}{\rho^{n+1}} \nabla \tilde{p}^{n+1} \approx \nabla \cdot \frac{1}{\overline{\rho}^{n+1}} \nabla \tilde{p}^{n+1} + \nabla \cdot \left(\frac{1}{\rho^{n+1}} - \frac{1}{\overline{\rho}^{n+1}} \right) \nabla \tilde{p}^n. \tag{6.3}$$

The first term on the right hand side of (6.3) is absorbed in $\nabla^2 \mathcal{H}$. In the second term, which becomes part of $\nabla \cdot \mathbf{F}$, we must use the most recent value of the pressure $\tilde{p}^n$. The expression $\overline{\rho}$ is an average density, equal to $2\rho_{min}\rho_{max}/(\rho_{min} + \rho_{max})$. To make this correction, simply include the statement `BAROCLINIC=.TRUE.` on the `MISC` line. The cost of the correction is not prohibitive – try calculations with and without the correction to determine if its inclusion is warranted.

In past versions of FDS, a DNS calculation (`DNS=.TRUE.` on the `MISC` line) included the baroclinic correction by default. However, starting with FDS 5.2, the correction must be explicitly invoked for both LES and DNS.

Example Case: helium_2d

This case demonstrates the use of baroclinic correction for an axially-symmetric helium plume. Note that the governing equations solved in FDS are written in terms of a three dimensional Cartesian coordinate system. However, a two dimensional Cartesian or two dimensional cylindrical (axially-symmetric) calculation can be performed by setting the number of cells in the y direction to 1. An example of an axially-symmetric helium plume is shown in Figure 6.5.

6.4.6 Special Topic: Stack Effect

Tall buildings often experience buoyancy-induced air movement due to temperature differences between inside and outside, known as *stack effect*. To simulate this phenomenon in FDS, you must include the entire

```
&HEAD CHID='helium_2d',TITLE='Axisymmetric Helium Plume' /
&MESH IJK=72,1,144 XB=0.00,0.08,-0.001,0.001,0.00,0.16, CYLINDRICAL=.TRUE. /
&TIME TWFIN=5.0 /
&MISC DNS=.TRUE., ISOTHERMAL=.TRUE., BAROCLINIC=.TRUE. /
&SPEC ID='HELIUM'  /
&SURF ID='HELIUM', VEL=-0.673, MASS_FRACTION(1)=1.0, TAU_MF(1)=0.3 /
&VENT MB='XMAX' ,SURF_ID='OPEN' /
&VENT MB='ZMAX' ,SURF_ID='OPEN' /
&OBST XB= 0.0,0.036,-0.001,0.001,0.00,0.02, SURF_IDS='HELIUM','INERT','INERT' /
&DUMP PLOT3D_QUANTITY(1)='PRESSURE',PLOT3D_QUANTITY(5)='HELIUM' /
&SLCF PBY=0.000,QUANTITY='DENSITY', VECTOR=.TRUE. /
&SLCF PBY=0.000,QUANTITY='HELIUM' /
&TAIL /
```

Figure 6.5: Simulation of a helium plume.

building, or a substantial fraction of it, both inside and out, in the computational domain. It is important to capture the pressure and density decrease in the atmosphere based on the specified temperature LAPSE_RATE (°C/m) that is entered on the MISC line. Experiment with different meshing strategies before including any fire or HVAC functionality. Slowly build in complexity.

Example Case: stack_effect

If the interior temperature of a building is at a different temperature than the surrounding atmosphere, upward or downward air flows within shafts or stairwells connected to the ambient via leakage paths will occur. This phenomena is known as the *stack effect*. The **stack_effect** test case is a 2D simulation of a 304 m tall building initialized to a temperature of 20 °C with the surrounding ambient temperature initialized to 10 °C. Two small openings in the building are defined 2.5 m above the ground floor of the building and 2.5 m below the roof of the building. The initial density stratification is defined by assuming a lapse rate of 0 °C/m.

$$\rho_0(z) = \rho_\infty \, e^{\frac{gW}{\mathcal{R}_0 T_0} z} \tag{6.4}$$

Applying this to the external and internal locations at the lower and upper vents results in densities of 1.2392, 1.1969, 1.1954, and 1.1546 kg/m^3, respectively. FDS computes the same values to within machine precision. Since the openings in the building are equally spaced over its height, the neutral plane of the building will be close to its midpoint. The pressure gradient across the building's wall can be computed as

$$\delta P = \frac{W P_0 g}{R_0} \left(\frac{1}{T_{ambient}} - \frac{1}{T_{building}} \right) h \tag{6.5}$$

where h is the distance from the neutral plane. Using this pressure gradient in Bernoulli's equation (and assuming it remains constant) results in a velocity of 10.09 m/s through the vent. FDS computes a peak velocity of 10.13 m/s, an error of 0.5 %.

6.4.7 Special Topic: Large Eddy Simulation Parameters

In default mode, FDS uses the Smagorinsky form of Large Eddy Simulation (LES) to model subgrid-scale turbulence. The viscosity μ is modeled

$$\mu_{\text{LES}} = \rho \, (C_s \Delta)^2 \left(2 \, \bar{\mathbf{S}}_{ij} \cdot \bar{\mathbf{S}}_{ij} - \frac{2}{3} (\nabla \cdot \bar{\mathbf{u}})^2 \right)^{\frac{1}{2}} \tag{6.6}$$

where C_s is an empirical constant and Δ is a length on the order of the size of a grid cell. The bar above the various quantities denotes that these are the resolved, or *filtered*, values, meaning that they are computed on a numerical grid. The other diffusive parameters, the thermal conductivity and material diffusivity, are related to the turbulent viscosity by

$$k_{\text{LES}} = \frac{\mu_{\text{LES}} c_p}{\text{Pr}_t} \quad ; \quad (\rho D)_{l,\text{LES}} = \frac{\mu_{\text{LES}}}{\text{Sc}_t} \tag{6.7}$$

The turbulent Prandtl number Pr_t and the turbulent Schmidt number Sc_t are assumed to be constant for a given scenario. Although it is not recommended for most calculations, you can modify $C_s = 0.2$, $\text{Pr}_t = 0.5$, and $\text{Sc}_t = 0.5$ via the parameters CSMAG, PR, and SC on the MISC line. A more detailed discussion of these parameters is given in the FDS Technical Reference Guide [5].

6.4.8 Special Topic: Numerical Stability Parameters

The time step of an FDS simulation is constrained by the convective and diffusive transport speeds via two conditions. The first is known as the Courant-Friedrichs-Lewy (CFL) condition. The CFL condition asserts that the solution of the equations cannot be updated with a time step larger than that which would allow a parcel of fluid to travel further than a single mesh cell. In each mesh cell of dimension δx by δy by δz with velocity components u, v, and w, the CFL number is defined:

$$\text{CFL} = \delta t \, \max \left(\frac{|u|}{\delta x}, \frac{|v|}{\delta y}, \frac{|w|}{\delta z} \right) \tag{6.8}$$

Every time step, the CFL number is computed in each mesh cell, and the time step, δt, is adjusted if the maximum value of the CFL number is not between CFL_MIN and CFL_MAX, whose default values are 0.8 and 1.0, respectively. These values are included in the MISC namelist group.

A similar condition, but one constraining the time step when diffusive transport dominates, is sometimes called the Von Neumann condition. The Von Neumann number is defined:

$$\text{VN} = 2 \max \left(\nu, D, \frac{k}{\rho c_p} \right) \delta t \left(\frac{1}{\delta x^2} + \frac{1}{\delta y^2} + \frac{1}{\delta z^2} \right) \tag{6.9}$$

Like the CFL number, VN is computed in each mesh cell, and the time step is adjusted if VN is outside the range between VN_MIN and VN_MAX, which are 0.8 and 1.0 by default. Note that this constraint is applied to the momentum, mass and energy equations via the relevant diffusion parameter – viscosity, material diffusivity or thermal conductivity. This constraint on the time step is typical of any explicit, second-order numerical scheme for solving a parabolic partial differential equation. To save CPU time, the Von Neumann criterion is only invoked for DNS calculations or for LES calculations with mesh cells smaller than 5 mm.

Resetting the stability parameters is not recommended except in very special circumstances, as they can lead to simulations failing due to numerical instabilities.

If you want to prevent FDS from automatically changing the time step, set LOCK_TIME_STEP=.TRUE. on the TIME line, in which case the specified time step, DT, will not be adjusted. This parameter is intended for diagnostic purposes only, for example, timing program execution. It can lead to numerical instabilities if the initial time step is set too high.

6.5 Special Topic: Unusual Initial Conditions: The INIT Namelist Group (Table 15.8)

Usually, an FDS simulation begins at time $t = 0$ with ambient conditions. The air temperature is assumed constant with height, and the density and pressure decrease with height (the z direction). This decrease is not noticed in most building scale calculations, but it is important in large outdoor simulations. There are some scenarios for which it is convenient to change the ambient conditions within some rectangular region of the domain. If so, add lines of the form

```
&INIT XB=0.5,0.8,2.1,3.4,2.5,3.6, TEMPERATURE=30. /
```

Here, within the region whose bounds are given by the sextuplet XB, the initial temperature shall be 30 °C instead of the ambient. This construct can also be used for DENSITY or MASS_FRACTION(N) where N indicates the Nth species listed in the input file. Make sure that you specify all species (components of MASS_FRACTION(N)) on the same INIT line.

The INIT construct may be useful in examining the influence of stack effect in a building, where the temperature is different inside and out.

Note that a solid obstruction can be given an initial temperature via the parameter TMP_INNER on the SURF line. An initial velocity can be prescribed via U0, V0, and W0 on the MISC line.

6.6 Special Topic: Setting Limits: The CLIP Namelist Group (Table 15.2)

On rare occasions you might need to set upper or lower bounds on the density, temperature, or species mass fractions. The parameters listed in Table 15.2 are for diagnostic purposes only.

Chapter 7

Building the Model

A considerable amount of work in setting up a calculation lies in specifying the geometry of the space to be modeled and applying boundary conditions to these objects. The geometry is described in terms of rectangular obstructions that can heat up, burn, conduct heat, *etc.*; and vents from which air or fuel can be either injected into, or drawn from, the flow domain. A boundary condition needs to be assigned to each obstruction and vent describing its thermal properties. A fire is just one type of boundary condition. This chapter describes how to build the model.

7.1 Bounding Surfaces: The `SURF` Namelist Group (Table 15.23)

Before describing how to build up the geometry, it is first necessary to explain how to describe what these bounding surfaces consist of. `SURF` is the namelist group that defines the structure of all solid surfaces or openings within or bounding the flow domain. Boundary conditions for obstructions and vents are prescribed by referencing the appropriate `SURF` line(s) whose parameters are described in this section.

The default boundary condition for all solid surfaces is that of a inert wall with the temperature fixed at `TMPA`, and is referred to as `'INERT'`. If only this boundary condition is needed, there is no need to add any `SURF` lines to the input file. If additional boundary conditions are desired, they are to be listed one boundary condition at a time. Each `SURF` line consists of an identification string `ID='...'` to allow references to it by an obstruction or vent. Thus, on each `OBST` and `VENT` line that are to be described below, the character string `SURF_ID='...'` indicates the `ID` of the `SURF` line containing the desired boundary condition parameters. If a particular `SURF` line is to be applied as the default boundary condition, `CONCRETE` for example, set `SURF_DEFAULT='CONCRETE'` on the `MISC` line.

7.2 Creating Obstructions: The `OBST` Namelist Group (Table 15.14)

The namelist group `OBST` contains parameters used to define obstructions. The entire geometry of the model is made up entirely of rectangular solids, each one introduced on a single line in the input file.

7.2.1 Basics

Each `OBST` line contains the coordinates of a rectangular solid within the flow domain. This solid is defined by two points (x_1, y_1, z_1) and (x_2, y_2, z_2) that are entered on the `OBST` line in terms of the sextuplet
`XB = X1, X2, Y1, Y2, Z1, Z2`
In addition to the coordinates, the boundary conditions for the obstruction can be specified with the parameter `SURF_ID`, which designates which `SURF` group (Section 7.1) to apply at the surface of the obstruction.

If the obstruction has different properties for its top, sides and bottom, do not specify only one `SURF_ID`. Instead, use `SURF_IDS`, an array of three character strings specifying the boundary condition `ID`s for the top, sides and bottom of the obstruction, respectively. If the default boundary condition is desired, then `SURF_ID(S)` need not be set. However, if at least one of the surface conditions for an obstruction is the inert default, it can be referred to as `'INERT'`, but it does not have to be explicitly defined. For example:

```
&SURF ID='FIRE',HRRPUA=1000.0 /
&OBST XB=2.3,4.5,1.3,4.8,0.0,9.2,SURF_IDS='FIRE','INERT','INERT' /
```

puts a fire on top of the obstruction. This is a simple way of prescribing a burner.

Some additional features of obstructions are as follows:

- In addition to `SURF_ID` and `SURF_IDS`, you can also use the sextuplet `SURF_ID6` as follows:

  ```
  &OBST XB=2.3,4.5,1.3,4.8,0.0,9.2,
        SURF_ID6='FIRE','INERT','HOT','COLD','BLOW','INERT' /
  ```

  where the six surface descriptors refer to the planes $x = 2.3$, $x = 4.5$, $y = 1.3$, $y = 4.8$, $z = 0.0$, and $z = 9.2$, respectively. Note that `SURF_ID6` should not be used on the same `OBST` line as `SURF_ID` or `SURF_IDS`.

- Obstructions can have zero thickness. Often, thin sheets, like a window, form a barrier, but if the numerical mesh is coarse relative to the thickness of the barrier, the obstruction might be unnecessarily large if it is assumed to be one layer of mesh cells thick. All faces of an obstruction are shifted to the closest mesh cell. If the obstruction is very thin, the two faces may be approximated on the same cell face. FDS and Smokeview render this obstruction as a thin sheet, but it is allowed to have thermally thick boundary conditions. This feature is fragile, especially in terms of burning and blowing gas. A thin sheet obstruction can only have one velocity vector on its face, thus a gas cannot be injected reliably from a thin obstruction because whatever is pushed from one side is necessarily pulled from the other. For full functionality, the obstruction should be specified to be at least one mesh cell thick. Thin sheet obstructions work fine as flow barriers, but other features are fragile and should be used with caution. To prevent FDS from allowing thin sheet obstructions, set `THICKEN_OBSTRUCTIONS=.TRUE.` on the `MISC` line, or `THICKEN=.TRUE.` on each `OBST` line for which the thin sheet assumption is not allowed.

- Unlike earlier versions of FDS, obstructions that are too small relative to the underlying numerical mesh are rejected. Be careful when testing cases on coarse meshes.

- Obstructions may be created or removed during a simulation. See Section 13.4.1 for details.

- If two obstructions overlap at one or more faces, the one listed last in the input file takes precedence over the one listed first, in the sense that the latter's surface properties will be applied to the overlapping face. Smokeview renders both obstructions independently of each other, often leading to an unsightly cross-hatching of the two surface colors where there is an overlap. A simple remedy for this is to "shrink" the first obstruction slightly by adjusting its coordinates (`XB`) accordingly. Then, in Smokeview, toggle the "q" key to show the obstructions as you specified them, rather than as FDS rendered them.

- Obstructions can be protected from the `HOLE` punching feature. Sometimes it is convenient to create a door or window using a `HOLE`. For example, suppose a `HOLE` is punched in a wall to represent a door or window. An obstruction can be defined to fill this hole (presumably to be removed or colored differently or whatever) so long as the phrase `PERMIT_HOLE=.FALSE.` is included on the `OBST`

line. In general, any `OBSTruction` can be made impenetrable to a `HOLE` using this phrase. By default, `PERMIT_HOLE=.TRUE.`, meaning that an `OBSTruction` is assumed to be penetrable unless otherwise directed. Note that if an penetrable `OBSTruction` and an inpentetrable `OBSTruction` overlap, the `OBSTruction` with `PERMIT_HOLE=.FALSE.` should be listed first.

- If the obstruction is not to be removed or rejected for any reason, set `REMOVABLE=.FALSE.` This is sometimes needed to stop FDS from removing the obstruction if it is embedded within another, like a door within a wall.

- In rare cases, you might not want to allow a `VENT` to be attached to a particular obstruction, in which case set `ALLOW_VENT=.FALSE.`

- Obstructions can be made semi-transparent by assigning a `TRANSPARENCY` on the `OBST` line. This real parameter ranges from 0 to 1, with 0 being fully transparent. The parameter should always be set along with either `COLOR` or an `RGB` triplet. It can also be specified on the appropriate `SURF` line, along with a color indicator.

- Obstructions are drawn solid in Smokeview. To draw an outline representation, set `OUTLINE=.TRUE.`

7.2.2 Repeated Obstructions: The `MULT` Namelist Group (Table 15.13)

Sometimes obstructions are repeated over and over in the input file. This can be tedious to create and make the input file hard to read. However, if a particular obstruction or set of obstructions repeats itself in a regular pattern, you can use a utility known as a multiplier. If you want to repeat an obstruction, create a line in the input file as follows:

```
&MULT ID='m1', DX=1.2, DY=2.4, I_LOWER=-2, I_UPPER=3, J_LOWER=0, J_UPPER=5 /

&OBST XB=..., MULT_ID='m1' /
```

This has the effect of making an array of obstructions according to the following formulae:

$$x_i = x_0 + \delta x_0 + i\,\delta x \quad ; \quad \texttt{I\_LOWER} \le i \le \texttt{I\_UPPER}$$
$$y_j = y_0 + \delta y_0 + j\,\delta y \quad ; \quad \texttt{J\_LOWER} \le j \le \texttt{J\_UPPER}$$

Note that the same rules apply for the *z* direction as well. In situations where the position of the obstruction needs shifting prior to the multiplication, use the parameters `DX0`, `DY0`, and `DZ0`.

A generalization of this idea is to replace the parameters, `DX`, `DY`, and `DZ`, with a sextuplet called `DXB`. The six entries in `DXB` increment the respective values of the obstruction coordinates given by `XB`. For example, define the lower *y* bound of the original obstruction by `XB(3,0)`. The *n*th obstruction would be:

```
XB(3,N) = XB(3,0) + N*DXB(3)
```

Notice that we use `N_LOWER` and `N_UPPER` to denote the range of `N`. This more flexible input scheme allows you to create, for example, a slanted roof in which the individual roof segments shorten as they ascend to the top. This feature is demonstrated by the following short input file that creates a hollowed out pyramid using the four perimeter obstructions that form the outline of its base:

```
&HEAD CHID='pyramid', TITLE='Simple demo of multiplier function' /
&MESH IJK=100,100,100, XB=0.0,1.0,0.0,1.0,0.0,1.0 /
&TIME T_END=0. /
&MULT ID='south', DXB=0.01,-.01,0.01,0.01,0.01,0.01, N_LOWER=0, N_UPPER=39 /
```
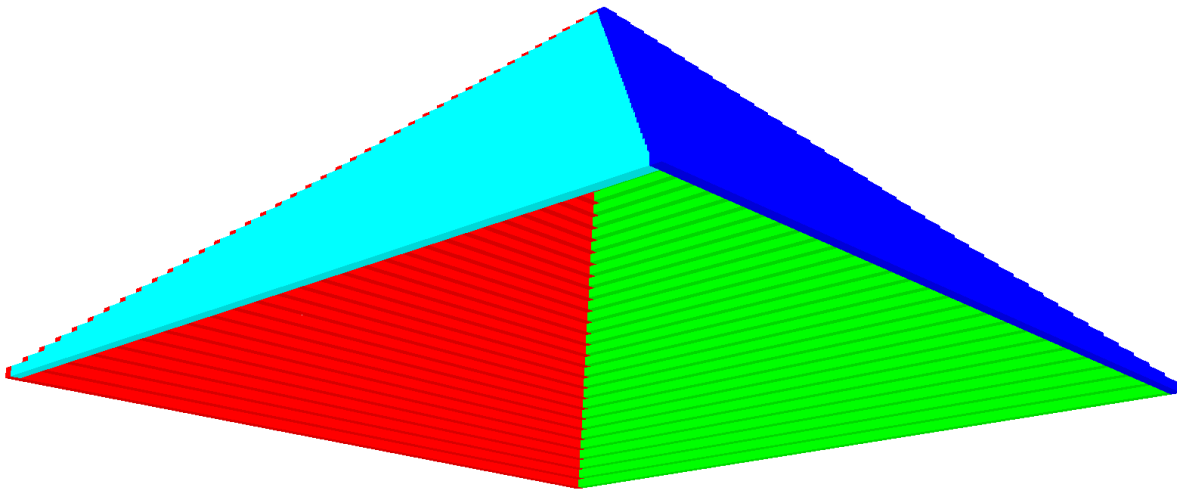
Figure 7.1: An example of the multiplier function.

```
&MULT ID='north', DXB=0.01,-.01,-.01,-.01,0.01,0.01, N_LOWER=0, N_UPPER=39 /
&MULT ID='east',  DXB=-.01,-.01,0.01,-.01,0.01,0.01, N_LOWER=0, N_UPPER=39 /
&MULT ID='west',  DXB=0.01,0.01,0.01,-.01,0.01,0.01, N_LOWER=0, N_UPPER=39 /
&OBST XB=0.10,0.90,0.10,0.11,0.10,0.11, MULT_ID='south', COLOR='RED' /
&OBST XB=0.10,0.90,0.89,0.90,0.10,0.11, MULT_ID='north', COLOR='BLUE' /
&OBST XB=0.10,0.11,0.11,0.89,0.10,0.11, MULT_ID='west',  COLOR='GREEN' /
&OBST XB=0.89,0.90,0.11,0.89,0.10,0.11, MULT_ID='east',  COLOR='CYAN' /
```

The end result of this input file is to create a pyramid by repeating long, rectangular obstructions at the base of each face in a stair-step pattern. Note in this case the use of N_LOWER and N_UPPER which automatically cause FDS to repeat the obstructions in sequence rather than as an array.

Note that the MULTiplication functionality works for MESHes, as well, but it only applies to the bounds (XB) of the mesh, not the number of cells.

7.2.3 Non-rectangular Geometry and Sloped Ceilings

The efficiency of FDS is due to the simplicity of its numerical mesh. However, there are situations in which certain geometric features do not conform to the rectangular mesh, such as a sloped ceiling or roof. In these cases, construct the curved geometry using rectangular obstructions, a process sometimes called "stair-stepping". A concern is that the stair-stepping changes the flow pattern near the wall. To lessen the impact of stair-stepping on the flow field near the wall, prescribe the parameter SAWTOOTH=.FALSE. on each OBST line that makes up the stair-stepped obstruction. The effect of this parameter is to prevent vorticity from being generated at sharp corners, in effect smoothing out the jagged steps that make up the obstruction. This is not a complete solution of the problem, but it does provide a simple way of ensuring that the flow field around a non-rectangular obstruction is not inhibited by extra drag created at sharp corners.

Do not apply SAWTOOTH=.FALSE. to obstructions that have any SURF_IDs with the attribute BURN_AWAY=.TRUE.

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Example Case: sawtooth

In this example, we look at the flow field past a diagonally oriented obstruction. If `SAWTOOTH=.FALSE.`, then the velocity boundary conditions will be applied in such a way as to minimize the impact of the boundaries due to vortices at sharp corners, as shown in the following example:

```
&OBST XB= 0.00, 0.05,-0.01, 0.01, 0.00, 0.05, SAWTOOTH=.FALSE., COLOR='EMERALD GREEN' /
&OBST XB= 0.05, 0.10,-0.01, 0.01, 0.00, 0.10, SAWTOOTH=.FALSE., COLOR='EMERALD GREEN' /
&OBST XB= 0.10, 0.15,-0.01, 0.01, 0.05, 0.15, SAWTOOTH=.FALSE., COLOR='EMERALD GREEN' /
&OBST XB= 0.15, 0.20,-0.01, 0.01, 0.10, 0.20, SAWTOOTH=.FALSE., COLOR='EMERALD GREEN' /
```

In Figure 7.2, the top set of obstructions are using the default `SAWTOOTH=.TRUE.` and the bottom set of obstructions are using `SAWTOOTH=.FALSE.` The adjacent obstructions that have `SAWTOOTH=.FALSE.` are displayed in Smokeview as one smooth obstruction, shown in green. Notice that as the air moves across the different sets of obstructions, the air velocity on the bottom set of obstructions is not affected as much by the vortices.
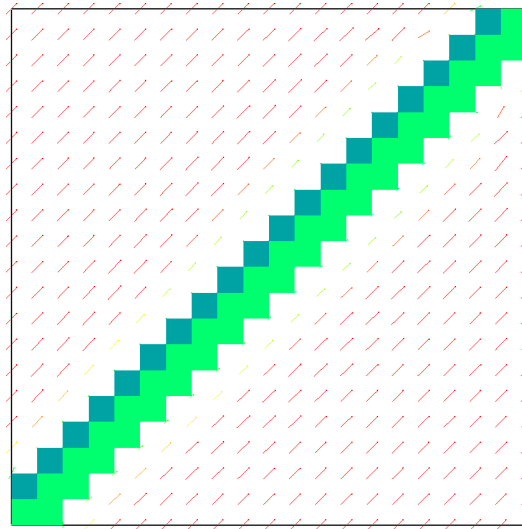
Figure 7.2: Simple example of `SAWTOOTH=.FALSE.`

7.3 Creating Voids: The `HOLE` Namelist Group (Table 15.7)

The `HOLE` namelist group is used to define parameters (Table 15.7) to carve a hole out of an existing obstruction or set of obstructions. To do this, add lines of the form

```
&HOLE XB=2.0,4.5,1.9,4.8,0.0,9.2 /
```

Any solid mesh cells within the volume $2.0 < x < 4.5$, $1.9 < y < 4.8$, $0.0 < z < 9.2$ are removed. Obstructions intersecting the volume are broken up into smaller blocks.

> If the hole represents a door or window, a good rule of thumb is to punch more than enough to create the hole. This ensures that the hole is created through the entire obstruction.

For example, if the `OBST` line denotes a wall 0.1 m thick:

```
&OBST XB=1.0,1.1,0.0,5.0,0.0,3.0 /
```

and you want to create a door, add this:

```
&HOLE XB=0.99,1.11,2.0,3.0,0.0,2.0 /
```

The extra centimeter added to the x coordinates of the hole make it clear that the hole is to punch through the entire obstruction.

When a `HOLE` is created, the affected obstruction(s) are either rejected, or created or removed at predetermined times. See Section 13.4.1 for details. To allow a hole to be controlled with either the `CTRL` or `DEVC` namelist groups, you will need to add the `CTRL_ID` or `DEVC_ID` parameter respectively, to the `HOLE` line.

If you want the obstruction that is to be cut out to have a different color than the original obstruction, set the `COLOR` or integer triplet `RGB` on the `HOLE` line (see Section 7.5).

When a `HOLE` is in a `.FALSE.` state, an obstruction is placed in the hole. To make this obstruction transparent, the `TRANSPARENCY` parameter should be specified by a real number from 0 to 1. Note that if `TRANSPARENCY` is specified, then either a `COLOR` or `RGB` triplet ought to be specified as well. A `TRANSPARENCY` value near, but not equal to, zero can be used to simulate a window when the `HOLE`'s `INITIAL_STATE=.FALSE.` When the `DEVC` or `CTRL` is activated and changes the state of the hole to `.TRUE.`, the `HOLE` is then open and completely transparent. See Section 13.4.1 for an example.

If an obstruction is not to be punctured by a `HOLE`, add `PERMIT_HOLE=.FALSE.` to the `OBST` line.

> It is a good idea to inspect the geometry by running either a setup job (`T_END=0` on the `TIME` line) or a short-time job to test the operation of devices and control functions.

> Note that a `HOLE` has no effect on a `VENT` or a mesh boundary. It only applies to `OBST`structions.

7.4   Applying Surface Properties: The VENT Namelist Group (Table 15.27)

Whereas the OBST group is used to specify obstructions within the computational domain, the VENT group (Table 15.27) is used to prescribe planes adjacent to obstructions or external walls. Note that the label VENT is used for historical reasons – this group of parameters has evolved well beyond its initial role as simply allowing for air to be blown into, or sucked out of, the computational domain.

7.4.1   Basics

The vents are chosen in a similar manner to the obstructions, with the sextuplet XB denoting a plane abutting a solid surface. Two of the six coordinates must be the same, denoting a plane as opposed to a solid.

> Note that only one VENT may be specified for any given wall cell. If additional VENT lines are specified for a given wall cell, FDS will output a warning message and ignore the subsequent lines (i.e. only the first vent will be applied)

The term "VENT" is somewhat misleading. Taken literally, a VENT can be used to model components of the ventilation system in a building, like a diffuser or a return. In these cases, the VENT coordinates form a plane on a solid surface forming the boundary of the duct. No holes need to be created through the solid; it is assumed that air is pushed out of or sucked into duct work within the wall. Less literally, a VENT is used simply as a means of applying a particular boundary condition to a rectangular patch on a solid surface. A fire, for example, is usually created by first generating a solid obstruction via an OBST line, and then specifying a VENT somewhere on one of the faces of the solid with a SURF_ID with the characteristics of the thermal and combustion properties of the fuel. For example, the lines

```
&OBST XB=0.0,5.0,2.0,3.0,0.0,4.0, SURF_ID='big block' /
&VENT XB=1.0,2.0,2.0,2.0,1.0,3.0, SURF_ID='hot patch' /
```

specify a large obstruction (with the properties given elsewhere in the file under the name 'big block') with a "patch" applied to one of its faces with alternative properties under the name 'hot patch'. This latter surface property need not actually be a "vent," like a supply or return duct, but rather just a patch with different boundary conditions than those assumed for the obstruction. Note that the surface properties of a VENT over-ride those of the underlying obstruction.

> Unlike previous versions of FDS, you can no longer specify a free-standing fan using the VENT construct. A VENT must always be attached to a solid obstruction. See Section 9.1 for instructions on specifying different types of fans.

An easy way to specify an entire external wall is to replace XB with MB (Mesh Boundary), a character string whose value is one of the following: 'XMAX', 'XMIN', 'YMAX', 'YMIN', 'ZMAX' or 'ZMIN' denoting the planes $x = $ XMAX, $x = $ XMIN, $y = $ YMAX, $y = $ YMIN, $z = $ ZMAX or $z = $ ZMIN, respectively. Like an obstruction, the boundary condition index of a vent is specified with SURF_ID, indicating which of the listed SURF lines to apply. If the default boundary condition is desired, then SURF_ID need not be set.

Be careful when using the MB shortcut when doing a multiple mesh simulation, that is, when more than one rectangular mesh is used. The plane designated by the keyword MB is applied to all of the meshes, possibly leading to confusion about whether a plane is a solid wall or an open boundary. Check the geometry in Smokeview to assure that the VENTs are properly prescribed. Use color as much as possible to double-check the set-up. More detail on color in Section 7.5 and Table 7.1. Also, the parameter OUTLINE=.TRUE. causes the VENT to be drawn as an outline in Smokeview.

7.4.2 Special `VENT`s

There are two reserved `SURF_ID`'s that may be applied to a `VENT` – `'OPEN'` and `'MIRROR'`. The term *reserved* means that these two `SURF_ID`s should not be explicitly defined by you. Their properties are predefined.

An `OPEN VENT`

The first special `VENT` is invoked by the parameter `SURF_ID='OPEN'`. This is used only if the `VENT` is applied to the exterior boundary of the computational domain, where it denotes a passive opening to the outside. By default, FDS assumes that the exterior boundary of the computational domain (the `XB`s on the `MESH` line) is a solid wall. To change this, use an `OPEN` vent as if it were an open door or window. To create a totally or partially open domain, use `OPEN` vents on the exterior mesh boundaries (`MB`s).

By default, it is assumed that ambient conditions exist beyond the `'OPEN'` vent. However, in some cases, you may want to alter this assumption, for example, the temperature. If you assume a temperature other than ambient, specify `TMP_EXTERIOR` along with `SURF_ID='OPEN'`. Use this option cautiously – in many situations if you want to describe the exterior of a building, it is better to include the exterior explicitly in your calculation because the flow in and out of the doors and windows will be more naturally captured. See Section 6.4.6 for more details.

As with exterior temperature, to change the exterior mass fraction of a particular gas species, set `MASS_FRACTION(N)` on the `VENT` line, where `N` denotes the species index. See Section 11.2 for more information about gas species.

If you want to specify a non-ambient pressure at the `OPEN` boundary, see Section 9.3.

> Starting with FDS 5.3.0, vents to the outside of the computational domain (`OPEN` vents) *can* be opened or closed during a simulation. It is best done by creating or removing a thin obstruction that covers the `OPEN VENT`. See Section 13.4.2 for details.

A `MIRROR VENT`

A `VENT` with `SURF_ID='MIRROR'` denotes a symmetry plane. Usually, a `MIRROR` spans an entire face of the computational domain, essentially doubling the size of the domain with the `MIRROR` acting as a plane of symmetry. The flow on the opposite side of the `MIRROR` is exactly reversed. From a numerical point of view, a `MIRROR` is a no-flux, free-slip boundary. As with `OPEN`, a `MIRROR` can only be prescribed at an exterior boundary of the computational domain. Often, `OPEN` or `MIRROR` `VENT`s are prescribed along an entire side of the computational domain, in which case the "`MB`" notation is handy.

> Note that the mirror image of a scene is **not** shown in Smokeview.

A word of warning about `MIRROR` boundaries in FDS. In conventional RANS (Reynolds-Averaged Navier-Stokes) models, symmetry boundaries are often used as a way of saving on computation time. However, because FDS is an LES (Large Eddy Simulation) model, the use of symmetry boundaries should be considered carefully. The reason for this is that an LES model does not compute a time-averaged solution of the N-S equations. In other words, for a RANS model, a fire plume is represented as an axially-symmetric flow field because that is what you would expect if you time-averaged the actual flow field over a sufficient amount of time. Thus, for a RANS model, a symmetry boundary along the plume centerline is appropriate. In an LES model, however, there is no time-averaging built into the equations, and there is no time-averaged,

symmetric solution. Putting a `MIRROR` boundary along the centerline of a fire plume will change its dynamics entirely. It will produce something very much like the flow field of a fire that is adjacent to a vertical wall. For this reason, a `MIRROR` boundary condition is not recommended along the centerline of a turbulent fire plume. If the fire or burner is very small, and the flow is laminar, then the `MIRROR` boundary condition makes sense. In fact, in 2-D calculations, `MIRROR` boundary conditions are employed in the third coordinate direction (this is done automatically, you need not specify it explicitly).

7.4.3 Controlling `VENT`s

`VENT` functionality can be controlled in some cases using "devices" and "controls," specified via a `DEVC_ID` or a `CTRL_ID`. See Section 13.4.2 for details.

7.4.4 Trouble-Shooting `VENT`s

Unlike most of the entries in the input file, the order that you specify `VENT`s can be important. There might be situations where it is convenient to position one `VENT` atop another. For example, suppose you want to designate the ceiling of a compartment to have a particular set of surface properties, and you designate the entire ceiling to have the appropriate `SURF_ID`. Then, you want to designate a smaller patch on the ceiling to have another set of surface properties, like an air supply. In this case, you must designate the supply `VENT` **first** because for that area of the ceiling, FDS will ignore the ceiling properties and apply the supply properties. FDS processes the first `VENT`, not the second as it did in versions prior to FDS 5. Now, the rule for `VENT`s is "first come, first served." Keep in mind, however, that the second `VENT` is not rejected entirely – only where there is overlap. FDS will also print out a warning to the screen (or to standard error) saying which `VENT` has priority.

Smokeview can help identify where two `VENT`s overlap, assuming each has a unique `COLOR`. Because Smokeview draws `VENT`s on top of each other, areas of overlap will have a grainy, awkward appearance that changes pattern as you move the scene. In situations where you desire the overlap for the sake of convenience, you might want to slightly adjust the coordinates of the preferred `VENT` so that it is slightly offset from the solid surface. Make the offset less than about a tenth of a cell dimension so that FDS snaps it to its desired location. Then, by toggling the "q" key in Smokeview, you can eliminate the grainy color overlap by showing the `VENT` exactly where you specified it, as opposed to where FDS repositioned it. This trick also works where the faces of two obstructions overlap.

If an error message appears requesting that the orientation of a vent be specified, first check to make sure that the vent is a plane. If the vent is a plane, then the orientation can be forced by specifying the parameter `IOR`. If the normal direction of the `VENT` is in the positive x direction, set `IOR=1`. If the normal direction is in the negative x direction, set `IOR=-1`. For the y and z direction, use the number 2 and 3, respectively. Setting `IOR` may sometimes solve the problem, but it is more likely that if there is an error message about orientation, then the `VENT` is buried within a solid obstruction, in which case the program cannot determine the direction in which the `VENT` is facing.

7.5 Coloring Obstructions, Vents, Surfaces and Meshes

Colors for many items within FDS can be prescribed in two ways; a triplet of integers after keyword `RGB` or one of many `COLOR` name character strings.

The three `RGB` integer numbers range from 0 to 255, indicating the amount of Red, Green and Blue that make up the color. If you define the `COLOR` by name, it is important that you type the name EXACTLY as it is listed in the color tables here in this document and on the FDS website.

Table 7.1 provides a small sampling of `RGB` values and `COLOR` names for a variety of colors. A complete listing of all 500+ colors that can be specified by name after the `COLOR` keyword is available on the FDS website. If the `COLOR` name is not listed in the table on the website, then that name does not exist to FDS.

It is highly recommended that colors be assigned to surfaces via the `SURF` line because as the geometries of FDS simulations become more complex, it is very useful to use color as a spot check to determine if the desired surface properties have been assigned throughout the room or building under study.

For example, if you desire that all surfaces associated with a given `SURF` line be colored the same way, prescribe a triplet of integers called `RGB` on the `SURF` line. The following `SURF` line;

```
&SURF ID='UPHOLSTERY',...,RGB=0,255,0 /
```

will cause the furnishings with a "SURF" of "UPHOLSTERY" to be colored green in Smokeview. It is best to avoid using the primary colors because these same colors are used by Smokeview to draw color contours.

Obstructions and vents may be colored individually (over-riding the `SURF` line's `RGB`) by specifying `COLOR` value to any of the listed names in Table 7.1 or `'INVISIBLE'` on the respective `OBST` or `VENT` line. Using `'INVISIBLE'` causes the vent or obstruction to not be drawn.

Colors may also be specified using the integer triplet `RGB` on an `OBST` or `VENT` line to gain a wider color palette. The use of `RGB` is preferable, especially to create colors that do not clash with the pastel colors used to show temperatures, concentrations, *etc.* See Table 7.1 for a list of color names and RGB values.

7.5.1 Texture Mapping

There are various ways of prescribing the color of various objects within the computational domain, but there is also a way of pasting images onto the obstructions for the purpose of making the Smokeview images more realistic. This technique is known as "texture mapping." For example, to apply a wood paneling image to a wall, add to the `SURF` line defining the physical properties of the paneling the text

```
&SURF ID='wood paneling',...,TEXTURE_MAP='paneling.jpg',TEXTURE_WIDTH=1.,
      TEXTURE_HEIGHT=2. /
```

Assuming that a JPEG file called **paneling.jpg** exists in the working directory, Smokeview should read it and display the image wherever the paneling is used (SGI Users: use rgb files instead of jpg). Note that the image does not appear when Smokeview is first invoked. It is an option controlled by the `Show/Hide` menu. The parameters `TEXTURE_WIDTH` and `TEXTURE_HEIGHT` are the physical dimensions of the image. In this case, the JPEG image is of a 1 m wide by 2 m high piece of paneling. Smokeview replicates the image as often as necessary to make it appear that the paneling is applied where desired. Consider carefully how the image repeats itself when applied in a scene. If the image has no obvious pattern, there is no problem with the image being repeated. If the image has an obvious direction, the real triplet `TEXTURE_ORIGIN` should be added to the `VENT` or `OBST` line to which a texture map should be applied. For example,

```
&OBST XB=1.0,2.0,3.0,4.0,5.0,7.0,SURF_ID='wood paneling',
      TEXTURE_ORIGIN=1.0,3.0,5.0 /
```

applies paneling to an obstruction whose dimensions are 1 m by 1 m by 2 m, such that the image of the paneling is positioned at the point (1.0,3.0,5.0). The default value of `TEXTURE_ORIGIN` is (0,0,0), and the global default can be changed by added a `TEXTURE_ORIGIN` statement to the `MISC` line.

Table 7.1: Sample of Color Definitions (A complete list is included on the website)

Name		R	G	B	Name		R	G	B
AQUAMARINE		127	255	212	MAROON		128	0	0
ANTIQUE WHITE		250	235	215	MELON		227	168	105
BEIGE		245	245	220	MIDNIGHT BLUE		25	25	112
BLACK		0	0	0	MINT		189	252	201
BLUE		0	0	255	NAVY		0	0	128
BLUE VIOLET		138	43	226	OLIVE		128	128	0
BRICK		156	102	31	OLIVE DRAB		107	142	35
BROWN		165	42	42	ORANGE		255	128	0
BURNT SIENNA		138	54	15	ORANGE RED		255	69	0
BURNT UMBER		138	51	36	ORCHID		218	112	214
CADET BLUE		95	158	160	PINK		255	192	203
CHOCOLATE		210	105	30	POWDER BLUE		176	224	230
COBALT		61	89	171	PURPLE		128	0	128
CORAL		255	127	80	RASPBERRY		135	38	87
CYAN		0	255	255	RED		255	0	0
DIMGRAY		105	105	105	ROYAL BLUE		65	105	225
EMERALD GREEN		0	201	87	SALMON		250	128	114
FIREBRICK		178	34	34	SANDY BROWN		244	164	96
FLESH		255	125	64	SEA GREEN		84	255	159
FOREST GREEN		34	139	34	SEPIA		94	38	18
GOLD		255	215	0	SIENNA		160	82	45
GOLDENROD		218	165	32	SILVER		192	192	192
GRAY		128	128	128	SKY BLUE		135	206	235
GREEN		0	255	0	SLATEBLUE		106	90	205
GREEN YELLOW		173	255	47	SLATE GRAY		112	128	144
HONEYDEW		240	255	240	SPRING GREEN		0	255	127
HOT PINK		255	105	180	STEEL BLUE		70	130	180
INDIAN RED		205	92	92	TAN		210	180	140
INDIGO		75	0	130	TEAL		0	128	128
IVORY		255	255	240	THISTLE		216	191	216
IVORY BLACK		41	36	33	TOMATO		255	99	71
KELLY GREEN		0	128	0	TURQUOISE		64	224	208
KHAKI		240	230	140	VIOLET		238	130	238
LAVENDER		230	230	250	VIOLET RED		208	32	144
LIME GREEN		50	205	50	WHITE		255	255	255
MAGENTA		255	0	255	YELLOW		255	255	0

Chapter 8

Fire and Thermal Boundary Conditions

This chapter describes how to specify the thermal properties of solid objects. **This is the most challenging part of setting up the simulation.** Why? First, for both real and simulated fires, the growth of the fire is very sensitive to the thermal properties of the surrounding materials. Second, even if all the material properties are known to some degree, the physical phenomena of interest may not be simulated properly due to limitations in the model algorithms or resolution of the numerical mesh. It is your responsibility to supply the thermal properties of the materials, and then assess the performance of the model to ensure that the phenomena of interest are being captured.

8.1 Basics

By default, the outer boundary of the computational domain is assumed to be a solid boundary that is maintained at ambient temperature. The same is true for any obstructions that are added to the scene. To specify the properties of solids, use the namelist group SURF (Section 7.1). Starting in FDS 5, solids are assumed to consist of layers which can be made of different materials. The properties of each material required are designated via the MATL namelist group (Section 8.2). These properties indicate how rapidly the materials heat up, and how they burn. Each MATL entry in the input file must have an ID, or name, so that they may be associated with a particular SURF via the parameter MATL_ID. For example, the input file entries:

```
&MATL ID             = 'BRICK'
      CONDUCTIVITY   = 0.69
      SPECIFIC_HEAT  = 0.84
      DENSITY        = 1600. /

&SURF ID        = 'BRICK WALL'
      MATL_ID   = 'BRICK'
      COLOR     = 'RED'
      BACKING   = 'EXPOSED'
      THICKNESS = 0.20 /

&OBST XB=0.1, 5.0, 1.0, 1.2, 0.0, 1.0, SURF_ID='BRICK WALL' /
```

define a brick wall that is 4.9 m long, 1 m high, and 20 cm thick.

The thickness of the wall indicated by the `OBST` line need not match that indicated by the `SURF` line. The thickness of the material on the surface of the wall is dictated by the parameter `THICKNESS`. These two parameters are independent for each other, the `OBST` line describes the overall geometric structure, the `SURF` line describes the characteristics of the surfaces of the geometry which includes the thickness of the layers of materials applied to that surface.

8.1.1 Simple Thermal Boundary Conditions

Usually, the thermal properties of a solid boundary are specified via the `MATL` namelist group, which is in turn invoked by the `SURF` entry via the character string `MATL_ID`. However, sometimes it is convenient to simply specify a fixed temperature boundary condition, in which case set `TMP_FRONT` to be the surface temperature in units of °C. One may also specify a fixed heat flux. Two methods are available to do this. The first is to specify a `NET_HEAT_FLUX` in units of kW/m^2. When this is specified FDS will compute the surface temperature required to ensure that the combine radiative and convective heat flux from the surface is equal to the `NET_HEAT_FLUX`. The second method is to specify separately the `CONVECTIVE_HEAT_FLUX`, in units of kW/m^2, and the radiative heat flux. The radiative heat flux is specified by setting both `TMP_FRONT` and `EMISSIVITY`. Note that if you wish there to be only a convective heat flux from a surface, then the `EMISSIVITY` should be set to zero. If `NET_HEAT_FLUX` or `CONVECTIVE_HEAT_FLUX` is positive, the wall heats up the surrounding gases. If `NET_HEAT_FLUX` or `CONVECTIVE_HEAT_FLUX` is negative, the wall cools the surrounding gases.

For some special applications, it is often desired that a solid surface be adiabatic, that is, there is no net heat transfer (radiative and convective) from the gas to the solid. For this case, all that must be prescribed on the `SURF` line is `ADIABATIC=.TRUE.`, nothing else. FDS will compute a wall temperature so that the sum of the convective and radiative fluxes is zero. Specifying a surface as `ADIABATIC` will result in FDS defining `NET_HEAT_FLUX=0`.

8.1.2 Fire with a Known Heat Release Rate

Solids and liquid fuels can be modeled by specifying their relevant properties via the `MATL` namelist group. However, if you simply want to specify a fire of a given heat release rate (HRR), you need not specify any material properties. A specified fire is basically modeled as the ejection of gaseous fuel from a solid surface or vent. This is essentially a burner, with a specified Heat Release Rate Per Unit Area, `HRRPUA`, in units of kW/m^2. For example

```
&SURF ID='FIRE',HRRPUA=500. /
```

applies 500 kW/m^2 to any surface with the attribute `SURF_ID='FIRE'`. See the discussion of **Time Dependent Conditions** in Section 10 to learn how to ramp the heat release rate up and down.

An alternative to `HRRPUA` with the exact same functionality is `MLRPUA`, except this parameter specifies the Mass Loss Rate of fuel gas Per Unit Area in kg/m^2/s. Do not specify both `HRRPUA` and `MLRPUA` on the same `SURF` line. With either, the stoichiometry of the gas phase reaction is set by the parameters on the `REAC` line. All of the species associated with the combustion process are accounted for by way of the mixture fraction variable and should not be explicitly prescribed. The exception to this rule is where a non-reacting gas is introduced into the domain that merely serves as a diluent, like CO_2 from an extinguisher or H_2O from evaporated sprinkler droplets (see Section 11.2 for details). If a finite rate combustion model is desired instead of the default mixture fraction model, see Section 11.2.4.

Specifying `HRRPUA` or `MLRPUA` automatically invokes the mixture fraction combustion model.

8.1.3 Special Topic: A Radially-Spreading Fire

Sometimes it is desired that a fire spread radially at some specified rate. Rather than trying to design material properties to achieve this, you can alternatively use a VENT in a special way. If the SURF_ID associated with a VENT defines a specified heat release rate, HRRPUA, and time history, RAMP_Q or TAU_Q, you can also specify XYZ and SPREAD_RATE on the VENT line. Then the fire is directed to start at the point XYZ and spread radially at a rate of SPREAD_RATE (m/s). The ramp-up begins at the time when the fire arrives at a given point. For example, the lines

```
&SURF ID='FIRE', HRRPUA=500.0, RAMP_Q='fireramp' /
&RAMP ID='fireramp', T= 0.0, F=0.0 /
&RAMP ID='fireramp', T= 1.0, F=1.0 /
&RAMP ID='fireramp', T=30.0, F=1.0 /
&RAMP ID='fireramp', T=31.0, F=0.0 /
&VENT XB=0.0,5.0,1.5,9.5,0.0,0.0, SURF_ID='FIRE', XYZ=1.5,4.0,0.0, SPREAD_RATE=0.03 /
```

create a rectangular patch at $z = 0$ on which the fire starts at the point (1.5,4.0,0.0) and spreads outwards at a rate of 0.03 m/s. Each surface cell burns for 30 s as the fire spreads outward, creating a widening ring of fire. Note that the RAMP_Q is used in this construct to turn the burning on and off to simulate the consumption of fuel as the fire spreads radially. It should not be used to mimic the "*t*-squared" curve – the whole point of the exercise is to mimic this curve in a more natural way. Eventually, the fire goes out as the ring grows past the boundary of the rectangle. Some trial and error is probably required to find the SPREAD_RATE that leads to a desired time history of the heat release rate.

8.2 Heat Conduction in Solids

Specified temperature or heat flux boundary conditions are easy to apply, but only of limited usefulness in real fire scenarios. In most cases, walls, ceilings and floors are made up of several layers of lining materials. The `MATL` namelist group is used to define the properties of the materials that make up boundary solid surfaces. A solid boundary can consist of multiple layers[1] of different materials, and each layer can consist of multiple material components.

8.2.1 Structure of Solid Boundaries

Material layers and components are specified on the `SURF` line via the array called `MATL_ID(IL,IC)`. The argument `IL` is an integer indicating the layer index, starting at 1, the layer at the exterior boundary. The argument `IC` is an integer indicating the component index. For example, `MATL_ID(2,3)='BRICK'` indicates that the third material component of the second layer is `BRICK`. In practice, the materials are often listed as in the following example:

```
&MATL ID            = 'INSULATOR'
      CONDUCTIVITY  = 0.041
      SPECIFIC_HEAT = 2.09
      DENSITY       = 229. /

&SURF ID        = 'BRICK WALL'
      MATL_ID   = 'BRICK','INSULATOR'
      COLOR     = 'RED'
      BACKING   = 'EXPOSED'
      THICKNESS = 0.20,0.10 /
```

Without arguments, the parameter `MATL_ID` is assumed to be a list of the materials in multiple layers, with each layer consisting of only a single material component.

> When a `SURF` is applied to the face of an `OBST`, the first `MATL_ID` is at the face of the `OBST`, with the other `MATL_ID`s being applied in succession with the final `MATL_ID` being applied on the opposite face of the `OBST`. If in the example above, `BRICK WALL` was applied to the entire `OBST` using `SURF_ID`, then when doing a heat transfer calculation from the +x face to the -x face, FDS would consider the `OBST` to be `BRICK` followed by `INSULATOR` and the same for a heat transfer calculation from the -x face to the +x face. To avoid this the user would need to specify a second `SURF` that has the reverse `MATL_ID` and use `SURF_ID6` to apply the two `SURF` definitions to opposite faces of the `OBST`.

Mixtures of solid materials within the same layer can be defined using the `MATL_MASS_FRACTION` keyword. This parameter has the same two indices as the `MATL_ID` keyword. For example, if the brick layer contains some additional water, the input could look like this:

```
&MATL ID            = 'WATER'
      CONDUCTIVITY  = 0.60
      SPECIFIC_HEAT = 4.19
      DENSITY       = 1000. /

&SURF ID                    = 'BRICK WALL'
      MATL_ID(1,1:2)        = 'BRICK','WATER'
```

---

[1]The maximum number of material layers is 20. The maximum number of material components is 20.

```
MATL_MASS_FRACTION(1,1:2) = 0.95,0.05
MATL_ID(2,1)              = 'INSULATOR'
COLOR                     = 'RED'
BACKING                   = 'EXPOSED'
THICKNESS                 = 0.20,0.10 /  <--- for layers 1 and 2
```

In this example, the first layer of material, Layer 1, is composed of a mixture of brick and water. This is given by the `MATL_ID` array which specifies Component 1 of Layer 1 to be brick, and Component 2 of Layer 1 to be water. The mass fraction of each is specified via `MATL_MASS_FRACTION`. In this case, brick is 95 %, by mass, of Layer 1, and water is 5 %.

It is important to notice that the components of the solid mixtures are treated as pure substances with no voids. The density of the mixture is

$$\rho = \left(\sum_i \frac{Y_i}{\rho_i} \right)^{-1} \tag{8.1}$$

where Y_i are the material mass fractions and ρ_i are the material bulk densities defined on the `MATL` lines. In the example above, the resulting density of the wall would be about 1553 kg/m^3. The fact that the wall density is smaller than the density of pure brick may be confusing, but can be explained easily. If the wall can contain water, the whole volume of the wall can not be pure brick. Instead there are voids (pores) that are filled with water. If the water is taken away, there is only about 1476 kg/m^3 of brick left. To have a density of 1600 kg/m^3 for a partially void wall, a higher density should be used for the pure brick.

8.2.2 Thermal Properties

For any solid material, specify its thermal `CONDUCTIVITY` (W/m·K), `DENSITY` (kg/m^3), `SPECIFIC_HEAT` (kJ/kg/K), and `EMISSIVITY` (0.9 by default). Both `CONDUCTIVITY` and `SPECIFIC_HEAT` can be functions of temperature. `DENSITY` and `EMISSIVITY` cannot. Temperature-dependence is specified using the `RAMP` convention. As an example, consider marinite, a wall material suitable for high temperature applications:

```
&MATL ID                 = 'MARINITE'
      EMISSIVITY         = 0.8
      DENSITY            = 737.
      SPECIFIC_HEAT_RAMP = 'c_ramp'
      CONDUCTIVITY_RAMP  = 'k_ramp' /
&RAMP ID='k_ramp', T= 24., F=0.13 /
&RAMP ID='k_ramp', T=149., F=0.12 /
&RAMP ID='k_ramp', T=538., F=0.12 /
&RAMP ID='c_ramp', T= 93., F=1.172 /
&RAMP ID='c_ramp', T=205., F=1.255 /
&RAMP ID='c_ramp', T=316., F=1.339 /
&RAMP ID='c_ramp', T=425., F=1.423 /
```

Notice that with temperature-dependent quantities, the `RAMP` parameter `T` means Temperature, and `F` is the value of either the specific heat or conductivity. In this case, neither `CONDUCTIVITY` nor `SPECIFIC_HEAT` is given on the `MATL` line, but rather the `RAMP` names.

Prior to FDS5, the thermal radiation from the gas space was always absorbed at the surface of the solid material and the emission to the gas space took place on the surface. Starting in FDS5, the solid material can be given an `ABSORPTION_COEFFICIENT` (1/m) that allows the radiation penetrate and absorb into the solid. Correspondingly, the emission of the material is based on the internal temperatures, not just the surface.

8.2.3 Back Side Boundary Conditions

The layers of a solid boundary are listed in the order from the surface to the interior. By default, this inner-most layer is assumed to back up to an air gap at ambient temperature. This is true even if the obstruction forms a wall in the model that backs up to another compartment. A good example of the default back side boundary condition is a sheet of gypsum board attached to wood studs. It is assumed that the back side of the gypsum board is an ambient temperature void space within the wall. It does not matter if the obstruction on which the boundary condition is applied is thick or thin.

There are other back side boundary conditions that can be applied. One is to assume that the wall backs up to an insulated material in which case no heat is lost to the backing material. The expression `BACKING='INSULATED'` on the `SURF` line prevents any heat loss from the back side of the material. Use of this condition means that you do not have to specify properties of the inner insulating material because it is assumed to be perfectly insulated.

If the wall is assumed to back up to the room on the other side of the wall and you want FDS to calculate the heat transfer through the wall into the space behind the wall, the attribute `BACKING='EXPOSED'` should be listed on the `SURF` line. This feature only works if the wall is less than or equal to one mesh cell thick, and if there is a non-zero volume of computational domain on the other side of the wall. Obviously, if the wall is an external boundary of the domain, the heat is lost to an ambient temperature void.

8.2.4 Initial and Back Side Temperature

By default, the initial temperature of the solid material is set to ambient (`TMPA` on the `MISC` line). Use `TMP_INNER` on the `SURF` line to specify a different initial temperature. Also, the back side temperature boundary condition of a solid can be set using the parameter `TMP_BACK` on the `SURF` line. `TMP_BACK` is not the actual back side surface temperature, but rather the gas temperature to which the back side surface is exposed. This parameter has no meaning for surfaces with `BACKING='EXPOSED'` or `BACKING='INSULATED'`.

Note that the parameters `TMP_INNER` and `TMP_BACK` are only meaningful for solids with specified `THICKNESS` and material properties (via the `MATL_ID` keyword).

8.2.5 Walls with Different Materials Front and Back

If you apply the attribute `BACKING='EXPOSED'` on a `SURF` line that is applied to a zero or one-cell thick obstruction, FDS calculates the heat conduction through the entire `THICKNESS` and it uses the gas phase temperature and heat flux on the front and back sides for boundary conditions. A redundant calculation is performed on the opposite side of the obstruction, so be careful how you specify multiple layers. If the layering is symmetric, the same `SURF` line can be applied to both sides. However, if the layering is not symmetric, you must create two separate `SURF` lines and apply one to each side. For example, a hollow box column that is made of steel and covered on the outside by a layer of insulation material and a layer of plastic on top of the insulation material, would have to be described with two `SURF` lines like the following:

```
&SURF ID              = 'COLUMN EXTERIOR'
      COLOR           = 'ANTIQUE WHITE'
      BACKING         = 'EXPOSED'
      MATL_ID(1:2,1)  = 'PLASTIC','INSULATION','STEEL'
      THICKNESS(1:2)  = 0.002,0.036,0.0063 /

&SURF ID              = 'COLUMN INTERIOR'
      COLOR           = 'BLACK'
      BACKING         = 'EXPOSED'
```

```
    MATL_ID(1:2,1)      = 'STEEL','INSULATION','PLASTIC'
    THICKNESS(1:2)      = 0.0063,0.036,0.002 /
```

If, in addition, the insulation material and plastic are combustible, and their burning properties are specified on the appropriate MATL lines, then you need to indicate which side of the column would generate the fuel vapor. In this case, the steel is impermeable; thus you should add the parameter LAYER_DIVIDE=2.0 to the SURF line labelled 'COLUMN EXTERIOR' to indicate that fuel vapors formed by the heating of the two first layers ('PLASTIC' and 'INSULATION') are to be driven out of that surface. You need to also specify LAYER_DIVIDE=0.0 on the SURF line labelled 'COLUMN INTERIOR' to indicate that no fuel vapors are to driven into the interior of the column. In fact, values from 0.0 to 1.0 would work equally because the material 'STEEL' would not generate any fuel vapors.

By default, LAYER_DIVIDE is 0.5 times the number of layers for surfaces with EXPOSED backing, and equal to the number of layers for other surfaces.

8.2.6 Special Topic: Non-Planar Walls and Targets

All obstructions in FDS are assumed to conform to the rectilinear mesh, and all bounding surfaces are assumed to be flat planes. However, many objects, like cables, pipes, and ducts, are not flat. Even though these objects have to be represented in FDS as "boxes," you can still perform the internal heat transfer calculation as if the object were really cylindrical or spherical. For example, the input lines:

```
&OBST XB=0.0,5.0,1.1,1.2,3.4,3.5, SURF_ID='CABLE' /
&SURF ID='CABLE', MATL_ID='PVC', GEOMETRY='CYLINDRICAL', THICKNESS=0.01 /
```

can be used to model a power cable that is 5 m long, cylindrical in cross section, 2 cm in diameter. The heat transfer calculation is still one-dimensional; that is, it is assumed that there is a uniform heat flux all about the object. This can be somewhat confusing because the cable is represented as an obstruction of square cross section, with a separate heat transfer calculation performed at each face, and no communication among the four faces. Obviously, this is not an ideal way to do solid phase heat transfer, but it does provide a reasonable bounding surface temperature for the gas phase calculation. More detailed assessment of a cable would require a two or three-dimensional heat conduction calculation, which is not included in FDS. Use GEOMETRY='SPHERICAL' to describe a spherical object.

8.2.7 Special Topic: Solid Phase Numerical Gridding Issues

To compute the temperature and reactions inside the solids, FDS solves the one-dimensional heat transfer equation numerically. The size of the mesh cells on the surface of the solid is automatically chosen using a rule that makes the cell size smaller than the square root of the material diffusivity ($k/\rho c$). By default, the solid mesh cells increase towards the middle of the material layer and are smallest on the layer boundaries.

The default parameters are usually appropriate for simple heat transfer calculations but sometimes the use of pyrolysis reactions makes the temperatures and burning rate fluctuate. The numerical stability of the solid phase solution may then be improved by making the mesh density more uniform inside the material and by making the mesh cells smaller. Adjustments may also be needed in case of extremely transient heat transfer situations. Use STRETCH_FACTOR=1. on the SURF line to have a perfectly uniform mesh. Values between 1 and 2 give different levels of stretching. The size of all the mesh cells can be scaled by setting CELL_SIZE_FACTOR less than 1.0. For example, CELL_SIZE_FACTOR=0.5 makes the mesh cells half the size. Setting WALL_INCREMENT=1 on the TIME line forces the solid phase temperatures to be solved on every time step.

If all the material components of the surface are reacting, and the pyrolysis reactions have no solid residue, the thickness of the surface is going to shrink when the surface reacts. The shrinking behavior

can be prevented in the numerical model by setting `SHRINK=.FALSE.` on the `SURF` line. However, setting `SHRINK=.FALSE.` may introduce numerical problems in the wall solver. When all the material of a shrinking surface is consumed but `BURN_AWAY` is not prescribed, the surface temperature is set to `TMP_BACK`, convective heat flux to zero and burning rate to zero.

See Section 8.4 for ways to check and improve the accuracy of the solid phase calculation.

8.3 Pyrolysis Models

FDS has several approaches for describing the pyrolysis of solids and liquids. The approach to take depends largely on the availability of material properties and the appropriateness of the underlying pyrolysis model. This section provides a description of the parameters that describe a burning solid material when the burning rate is known. In other words, you use these parameters to *specify* the burning rate.

8.3.1 Solid Fuels that Burn at a Specified Rate

Real objects, like furnishings, office equipment, and so on, are often difficult to describe via the `SURF` and `MATL` parameters. Sometimes the only information about a given object is its bulk thermal properties, its "ignition" temperature, and what its subsequent burning rate is, as a function of time from ignition. For this situation, add lines similar to the following:

```
&MATL ID                 = 'stuff'
      CONDUCTIVITY       = 0.1
      SPECIFIC_HEAT      = 1.0
      DENSITY            = 900.0 /

&SURF ID                 = 'my surface'
      COLOR              = 'GREEN'
      MATL_ID            = 'stuff'
      HRRPUA             = 1000.
      IGNITION_TEMPERATURE = 500.
      RAMP_Q             = 'fire_ramp'
      THICKNESS          = 0.01 /

&RAMP ID='fire_ramp', T=  0.0, F=0.0 /
&RAMP ID='fire_ramp', T= 10.0, F=1.0 /
&RAMP ID='fire_ramp', T=310.0, F=1.0 /
&RAMP ID='fire_ramp', T=320.0, F=0.0 /
```

An object with surface properties defined by `'my surface'` shall burn at a rate of 1000 kW/m^2 after a linear ramp-up of 10 s following its "ignition" when its surface temperature reaches 500 °C. Burning shall continue for 5 min, and then ramp-down in 10 s. Note that the time `T` in the `RAMP` means time from ignition. Note also that now the "ignition temperature" is a surface property, not material property.

After the surface has ignited, the heat transfer into the solid is still being solved but there is no coupling between the burning rate and the surface temperature. As a result, the surface temperature may increase too much. To account for the energy loss due to the vaporization of the solid fuel, `HEAT_OF_VAPORIZATION` can be specified for the surface. For example, when using the lines below, the net heat flux at the material surface is reduced by a factor 1000 kJ/kg times the instantaneous burning rate.

```
&SURF ID                 = 'my surface'
      COLOR              = 'GREEN'
      MATL_ID            = 'stuff'
      HRRPUA             = 1000.
      IGNITION_TEMPERATURE = 500.
      HEAT_OF_VAPORIZATION = 1000.
      RAMP_Q             = 'fire_ramp'
      THICKNESS          = 0.01 /
```

The parameters `HRRPUA`, `IGNITION_TEMPERATURE`, and `HEAT_OF_VAPORIZATION` are all telling FDS that you want to control the burning rate yourself, but you still want to simulate the heating up and "ignition" of the fuel. When these parameters appear on the `SURF` line, they are acting in concert. If `HRRPUA` appears

alone, the surface will begin burning at the start of the simulation, like a piloted burner. The addition of an `IGNITION_TEMPERATURE` delays burning until your specified temperature is reached. The addition of `HEAT_OF_VAPORIZATION` tells FDS to account for the energy used to vaporize the fuel. For any of these options, if a `MATL` line is invoked by a `SURF` line containing a specified `HRRPUA`, then that `MATL` ought to have only thermal properties. It should have no reaction parameters, product yields, and so on, like those described in the previous sections. By specifying `HRRPUA`, you are controlling the burning rate rather than letting the material pyrolyze based on the conditions of the surrounding environment.

8.3.2 Solid Fuels that do NOT Burn at a Specified Rate

This section describes the parameters that describe the reactions that occur within solid materials when they are burning. It is strongly recommended before reading this section that you read some background material on solid phase pyrolysis, for example "Thermal Decomposition of Polymers," by Hirschler and Morgan, or "Flaming Ignition of Solid Fuels," by Torero, both of which are in the 4th edition of the *SFPE Handbook of Fire Protection Engineering*.

The Reaction Mechanism

A solid surface in FDS can consist of multiple layers with multiple material components per layer. The material components are described via `MATL` lines and are specified on the `SURF` line that describes the structure of the solid. Each `MATL` can undergo several reactions that may occur at different temperatures. It may not undergo any – it may only just heat up. However, if it is to change form via one or more reactions, designate the number of reactions with the integer `N_REACTIONS`. It is very important that you designate `N_REACTIONS` or else FDS will ignore all parameters associated with reactions. Note that experimental evidence of multiple reactions does not imply that a single material is undergoing multiple reactions, but rather that multiple material components are undergoing individual reactions at distinct temperatures. Currently, the maximum number of reactions for each material is 10 and the chain of consecutive reactions may contain up to 20 steps.

For a given `MATL`, the *j*th reaction can produce a (single) solid whose name is `RESIDUE(j)`, plus water vapor, and/or fuel gas. For example, the evaporation of water from a solid material is described by the "reaction" that converts liquid water to water vapor. This reaction occurs in the neighborhood of 100 °C and produces only water vapor. It does not produce a solid `RESIDUE` nor fuel gas. However, a pyrolyzing solid might undergo a reaction that produces a solid `RESIDUE`, water vapor, *and* fuel gas, all as part of the single reaction step. This information is conveyed to FDS via the *yields*: `NU_RESIDUE(j)`, `NU_WATER(j)`, and `NU_FUEL(j)`, respectively. The integer `j` indicates to which reaction the parameters apply. If, like the evaporation of water, only water vapor is produced, set `NU_WATER(j)=1.0` and the other two to zero. The yields are all zero by default. If `NU_RESIDUE(j)` is non-zero, then you *must* indicate what the solid residue is via `RESIDUE(j)`, the `ID` of another `MATL` that is also listed in the input file. Ideally, the sum of the yields should add to 1, meaning that the mass of the reactant is conserved. However, there are times when it is convenient to have the yields sum to something less than one. For example, the spalling or ablation of concrete can be described as a "reaction" that consumes energy but does not produce any "product" because the concrete is assumed to have either fallen off the surface in chunks or pulverized powder. The concrete's mass is not conserved *in the model* because it has essentially disappeared from that particular surface. A more general way to specify gaseous yields is to use the parameter `NU_GAS`, as explained in Section 11.2.3.

The Reaction Rates

For each reaction that each material component undergoes you must specify kinetic parameters of the reaction rate. The general evolution equation for a material undergoing one or more reactions is:

$$\frac{\partial Y_{s,i}}{\partial t} = -\sum_{j=1}^{N_{r,i}} r_{ij} + \sum_{i'=1}^{N_m} \sum_{j=1}^{N_{r,i'}} \nu_{s,i'j}\, r_{i'j} \quad (i' \neq i) \quad ; \quad r_{ij} = A_{ij}\, Y_{s,i}^{n_{s,ij}} \exp\left(-\frac{E_{ij}}{RT_s}\right) \quad ; \quad Y_{s,i} = \left(\frac{\rho_{s,i}}{\rho_{s0}}\right) \quad (8.2)$$

The term, r_{ij}, defines the rate of reaction at the temperature, T_s, of the ith material undergoing its jth reaction. The second term on the right of the equation represents the contributions of other materials producing the ith material as a residue with a yield of $\nu_{s,i'j}$. This term is denoted by NU_RESIDUE(j) on the i'-th MATL line. $\rho_{s,i}$ is the density of the ith material component of the layer, defined as the mass of the ith material component divided by the volume of the layer. ρ_{s0} is the initial density of the layer. Thus, $Y_{s,i} = \rho_{s,i}/\rho_{s0}$ is a quantity that increases if the ith material component is produced as a residue of some other reaction, or decreases if the ith component decomposes. If the layer is composed of only one material, then $\rho_{s,i}/\rho_{s0}$ is initially 1. $n_{s,ij}$ is the reaction order and prescribed under the name N_S(j), and is 1 by default. If the value of n_s is not known, it is a good starting point to assume $n_s = 1$.

The pre-exponential factor, A_{ij}, is prescribed under the name A(j) on the MATL line of the ith material, with units of s^{-1}. E_{ij}, the activation energy, is prescribed via E(j) in units of kJ/kmol. Remember that 1 kcal is 4.184 kJ, and be careful with factors of 1000. For a given reaction, specify both A and E, or neither. Do not specify only one of these two parameters. Typically, these parameters only have meaning when both are derived from a common set of experiments, like TGA (Thermo-Gravimetric Analysis).

It is very important to keep in mind that A and E are not available for most real materials. If A and E are not known, there are several parameters that can be used by FDS to derive effective values. The most important parameter to specify in place of A and E is the REFERENCE_TEMPERATURE (°C). To understand this parameter, consider the plot shown in Fig. 8.1. These curves represent the results of a hypothetical TGA experiment. The Mass Fraction (blue curve) is the normalized density of the material which decreases as the sample is slowly heated, in this case at a rate of 5 K/min. The Reaction Rate (green curve) is the rate of change of the mass fraction as a function of time. Where this curve peaks is referred to in FDS as the REFERENCE_TEMPERATURE.[2] Note that the REFERENCE_TEMPERATURE is *not* the same as an ignition temperature, nor is it necessarily the surface temperature of the burning solid. Rather, it is simply the temperature at which the mass fraction of the material decreases at its maximum rate within the context of a TGA or similar experimental apparatus.

Two additional parameters can be specified along with REFERENCE_TEMPERATURE (T_p) to help to fine tune the shape of the reaction rate curve, assuming some sort of experiment has been done to indicate at what temperature, and over what temperature range, the reaction takes place. First, the HEATING_RATE ($\dot{T}$) is the rate at which the temperature of the TGA (or equivalent) test apparatus was increased, in units of K/min. Its default value is 5 K/min. In Fig. 8.1, the area under the green curve (Reaction Rate) is equal to the heating rate (in units of K/s). Second, the PYROLYSIS_RANGE (ΔT) is the approximate width (in degrees Celsius or Kelvin) of the green curve, assuming its shape to be roughly triangular. Its default value is 80 °C. Using these input parameters, an estimate is made of the peak reaction rate, r_p, from which E, then A, can

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[2]The term "reference temperature" is used simply to maintain backward compatibility with earlier versions of FDS.
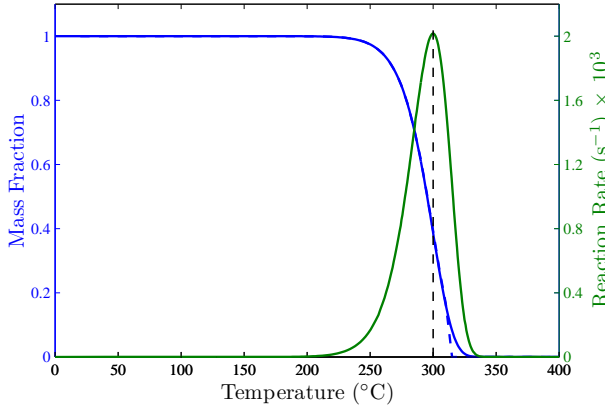
$$\frac{dY}{dt} = -AY \exp(-E/RT) \quad Y(0) = 1$$

$$\frac{dT}{dt} = \frac{5}{60} \frac{\text{K}}{\text{s}} \qquad T(0) = 20 + 273 \text{ K}$$

$$T_p = 300 + 273 \text{ K}$$
$$\Delta T = 80 \text{ K}$$
$$\nu_s = 0$$

Figure 8.1: The blue curve represents the normalized mass, $Y = \rho_s/\rho_{s0}$, of a solid material undergoing heating at a rate of 5 K/min. The green curve represents the reaction rate, $-dY/dt$. The system of ordinary differential equations that describe the transformation is shown at right. Note that the parameters T_p, ΔT, and ν_s represent the "reference" temperature, pyrolysis temperature range, and residue yield of the single reaction. From these parameters, values of A and E can be estimated using the formulae in Eqs. (8.3)-(8.5).

be calculated to ensure that the peak reaction rate occurs at the specified REFERENCE_TEMPERATURE. [3]

$$r_p = \frac{2\dot{T}}{\Delta T}(1 - \nu_s) \tag{8.3}$$

$$E = \frac{r_p}{Y_p}\frac{RT_p^2}{\dot{T}} \tag{8.4}$$

$$A = \frac{r_p}{Y_p}e^{E/RT_p} \tag{8.5}$$

In above, ν_r is the yield of solid residue and Y_p is the mass fraction (blue curve in Fig. 8.1) at the temperature where the reaction rate is its maximum. It is 0.4 by default and not adjustable. When in doubt about the values of these parameters, just specify the REFERENCE_TEMPERATURE. Note that FDS will automatically calculate A and E using the above formulas. Do not specify A and E if you specify REFERENCE_TEMPERATURE.

For the material decomposition shown in Fig. 8.1, the MATL would have the form:

```
&MATL ID                    = 'My Fuel'
      ...
      HEAT_OF_COMBUSTION        = ...
      N_REACTIONS               = 1
      NU_FUEL(1)                = 1.
      REFERENCE_TEMPERATURE(1)  = 300.
      HEAT_OF_REACTION(1)       = ... /
```

Note that the argument (1) has been added to the reaction parameters to emphasize the fact that these parameters are stored in arrays of length equal to N_REACTIONS. If there is only one reaction, you need not include the (1), but it is a good habit to get into. Note also that the HEAT_OF_COMBUSTION is the energy

---

[3]These formulas have been derived from an analysis that considers a first-order reaction. When using the proposed method, do not specify non-unity value for the reaction order N_S on the MATL line.

released per unit mass of fuel gas that mixes with oxygen and combusts. This has nothing to do with the pyrolysis process, so why is it specified here? The answer is that there can be only one *gas phase* reaction of fuel and oxygen in FDS, but there can be dozens of different materials and dozens of *solid phase* reactions. To ensure that the fuel vapors from different materials combust to produce the proper amount of energy, it is very important to specify a `HEAT_OF_COMBUSTION` for each material. That way, the mass loss rate of fuel gases is automatically adjusted so that the effective mass loss rate multiplied by the single, global, gas phase heat of combustion produces the expected heat release rate. If, for example, the `HEAT_OF_COMBUSTION` specified on the `REAC` line is twice that specified on the `MATL` line, the mass of contained within wall cell will be decremented by that determined by the pyrolysis model, but the mass added to gas phase would be reduced by 50 %. A different value of heat of combustion can be specified for each reaction and each gaseous species using the notation `HEAT_OF_COMBUSTION(j,s)`, as explained in Section 11.2.3.

Note that versions of FDS from 5.0 through 5.3 used a slightly different definition of `REFERENCE_TEMPERATURE` in addition to a parameter called `REFERENCE_RATE`. The latter has been removed and its use in FDS 5.4 and beyond will result in an immediate error message.

The solid phase reaction represented by Fig. 8.1 is very simple – a single, homogenous material is heated and gasified completely. In general, real materials are not so simple. First, they consist of more than one material component, each of which can react over a particular temperature interval, and some of which leave behind a solid residue. Some material components may even undergo multiple reactions that form different residues, like woods that form various amounts of tar, char, and ash, depending on the rate of heating. Figure 8.2 demonstrates a more complicated material than the one previously described. It is a hypothetical material that contains 10 % (by mass) water and 90 % solid material. The water evaporates in the neighborhood of 100 °C and the solid pyrolyzes in the neighborhood of 300 °C, leaving 20 % of its mass behind in the form of a solid residue.

The key input lines for this reaction are shown in Fig. 8.3. Note that the only parameters shown are those that describe the reaction mechanism, and that each of these parameters can be found either from visual inspection of the the mass loss (blue) curve or the reaction rate (green) curve. The thermal properties of each material would also be needed for an actual FDS simulation, but are not relevant in the context of a TGA or similar experiment that involves a slow heating of a small sample of material. The full set of parameters for these cases are listed in **pyrolysis_1.fds** and **pyrolysis_2.fds**. Those interested in testing potential solid phase reaction mechanisms ought to use these test cases as templates.
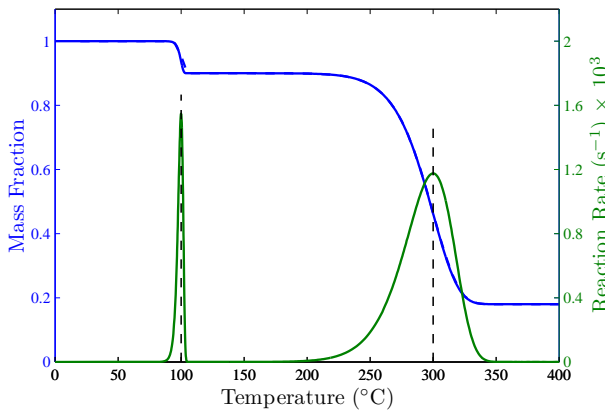
$$\frac{dY_1}{dt} = -A_{1,1} Y_1 \exp(-E_{1,1}/RT) \quad Y_1(0) = 0.1$$

$$\frac{dY_2}{dt} = -A_{2,1} Y_2 \exp(-E_{2,1}/RT) \quad Y_2(0) = 0.9$$

$$\frac{dY_3}{dt} = -\nu_{s,2,1} \frac{dY_2}{dt} \quad Y_3(0) = 0.0$$

$$\frac{dT}{dt} = \frac{5}{60} \frac{K}{s} \quad T(0) = 20 + 273 \text{ K}$$

$T_{p,1,1} = 100 + 273$ K	$T_{p,2,1} = 300 + 273$ K
$\Delta T_{1,2} = 10$ K	$\Delta T_{2,1} = 80$ K
$\nu_{s,1,1} = 0$	$\nu_{s,2,1} = 0.2$

Figure 8.2: The blue curve represents the combined mass fraction, $\sum Y_i$, and the green curve the net reaction rate, $-d/dt(\sum Y_i)$, for a material that contains 10 % water (by mass) that evaporates at a temperature of 100 °C, and 90 % solid material that pyrolyzes at 300 °C, leaving a 20 % (by mass) residue behind. Note that the numbered subscripts refer to the material component and the reaction, respectively. In this case, there are three material components, and the first two each undergo a single reaction. The third material component is formed as a residue of the reaction of the second material. The system of ordinary differential equations that governs the transformation of the materials is shown at right.

The Heat of Reaction

Equation (8.2) describes the rate of the reaction as a function of temperature. Most solid phase reactions require energy; that is, they are *endothermic*. The amount of energy consumed, per unit mass of reactant that is converted into something else, is specified by the HEAT_OF_REACTION(j). Technically, this is the enthalpy difference between the products and the reactant. A positive value indicates that the reaction is *endothermic*; that is, the reaction takes energy out of the system. Usually the HEAT_OF_REACTION is accurately known only for simple phase change reactions like the vaporization of water. For other reactions, it must be determined empirically.

Special Topic: The "Threshold" Temperature

In FDS, the reaction rate expression in Eq. (8.2) includes an optional term:

$$r_{ij} = A_{ij} Y_{s,i}^{n_{s,ij}} \exp\left(-\frac{E_{ij}}{RT_s}\right) \max\left[0, T_s - T_{thr,ij}\right]^{n_{t,ij}} \tag{8.6}$$

$T_{thr,ij}$ is an optional "threshold" temperature that allows the definition of non-Arrhenius pyrolysis functions and ignition criteria, and is prescribed by THRESHOLD_TEMPERATURE(j). By default, $T_{thr,ij}$ is -273.15 degrees Celsius, $n_{t,j}$ is zero; thus, the last term of Equation 8.6 does not affect the pyrolysis rate. The term can be used to describe a threshold temperature for the pyrolysis reaction by setting $T_{thr,ij}$ and $n_{t,j} = 0$. Then the term is equal to 0 at temperatures below $T_{thr,ij}$ and 1 at temperatures above. $n_{t,j}$ is prescribed under the name N_T(j).

```
&SURF ID                    = 'SAMPLE'
   ...
   MATL_ID(1,1:2)           = 'stuff', 'water'
   MATL_MASS_FRACTION(1,1:2) = 0.9,0.1 /

&MATL ID                 = 'water'
   ...
   N_REACTIONS           = 1
   REFERENCE_TEMPERATURE = 100.
   PYROLYSIS_RANGE       = 10.
   NU_WATER              = 1.
   HEAT_OF_REACTION      = ... /

&MATL ID                 = 'stuff'
   ...
   N_REACTIONS           = 1
   REFERENCE_TEMPERATURE = 300.
   PYROLYSIS_RANGE       = 80.
   NU_FUEL               = 0.8
   NU_RESIDUE            = 0.2
   RESIDUE               = 'ash'
   HEAT_OF_REACTION      = ... /

&MATL ID                 = 'ash'
      ... /
```

Figure 8.3: Input parameters for sample case **pyrolysis_2**.

8.3.3   Liquid Fuels

For a liquid fuel, the thermal properties are similar to those of a solid material, with a few exceptions. The evaporation rate of the fuel is governed by the Clausius-Clapeyron equation (see FDS Technical Reference Guide for details). The drawback of this approach is that the fuel mass flux is not an explicit function of temperature, but rather an iterative result depending on the temperature and flow conditions. To initiate the evaporation, an initial value of the fuel vapor volume flux is needed. If the initial value is (relatively) high, the evaporation starts regardless of any ignition source, and the the fuel begins burning at once.

Figure 8.4 contains the key input parameters to describe a steel pan filled with a thin layer of ethanol. Note that the material properties are not all traceable to a measurement.

The inclusion of BOILING_TEMPERATURE on the MATL line tells FDS to use its liquid pyrolysis model. It also automatically sets N_REACTIONS=1, that is, the only "reaction" is the phase change from liquid to gaseous fuel. Thus, HEAT_OF_REACTION in this case is the latent heat of vaporization. The gaseous fuel yield, NU_FUEL, is 0.97 instead of 1 to account for impurities in the liquid that do not take part in the combustion process.

The thermal conductivity, density and specific heat are used to compute the loss of heat into the liquid via conduction using the same one-dimensional heat transfer equation that is used for solids. Obviously, the convection of the liquid is important, but is not considered in the model.

The initial value of the fuel vapor volume flux can be specified using the parameter INITIAL_VAPOR_FLUX. Its default value is $5 \cdot 10^{-4}$ m^3/(sm^2).

Note also the ABSORPTION_COEFFICIENT for the liquid. This denotes the absorption in depth of thermal radiation. Liquids do not just absorb radiation at the surface, but rather over a thin layer near the surface. Its effect on the burning rate is significant.

```
&MATL ID                   = 'ETHANOL LIQUID'
      EMISSIVITY           = 1.0
      NU_FUEL              = 0.97
      HEAT_OF_REACTION     = 880.
      CONDUCTIVITY         = 0.17
      SPECIFIC_HEAT        = 2.45
      DENSITY              = 787.
      ABSORPTION_COEFFICIENT = 40.
      BOILING_TEMPERATURE  = 76. /

&MATL ID            = 'STEEL'
      EMISSIVITY    = 1.0
      DENSITY       = 7850.
      CONDUCTIVITY  = 45.8
      SPECIFIC_HEAT = 0.46 /

&MATL ID            = 'CONCRETE'
      DENSITY       = 2200.
      CONDUCTIVITY  = 1.2
      SPECIFIC_HEAT = 0.88 /

&SURF ID        = 'ETHANOL POOL'
      FYI       = '4 kg of ethanol in a 0.7 m x 0.8 m pan'
      COLOR     = 'YELLOW'
      MATL_ID   = 'ETHANOL LIQUID','STEEL','CONCRETE'
      THICKNESS = 0.0091,0.001,0.05
      TMP_INNER = 18. /
```

Figure 8.4: Input parameters for sample case **ethanol_pan**.

In the current implementation of the liquid fuel model, the evaporation rate is strongly grid dependent. Thus, it should be used with caution.

8.3.4 Fuel Burnout

The thermal properties of a solid or liquid fuel determine the length of time for which it can burn. In general, the burnout time is a function of the mass loss rate, $\dot{m}''$, the density, ρ_s, and the layer thickness, δ_s:

$$t_b = \frac{\rho_s \delta_s}{\dot{m}''} \tag{8.7}$$

However, each type of pyrolysis model handles fuel burnout in a slightly different way. These differences will be highlighted in the individual sections below.

Solid Fuel Burnout

If a heat release rate RAMP function is not included for a solid fuel that burns at a specified rate, the surface will continue to burn at the specified rate indefinitely with no fuel burnout. If detailed heat release rate versus time data is not available, you can estimate the burnout time for a surface using the heat of combustion, ΔH, material density, ρ_s, material thickness, δ_s, and HRRPUA, $\dot{q}''_f$:

$$t_b = \frac{\rho_s \delta_s \Delta H}{\dot{q}''_f} \tag{8.8}$$

Use the RAMP function to stop the burning once the calculated burnout time is reached.

The burnout time of a reacting solid fuel is calculated automatically by FDS based on the layer THICKNESS, component DENSITY, and the calculated burning rate.

Liquid Fuel Burnout

The burnout time of a liquid fuel is calculated automatically based on the liquid layer THICKNESS, liquid DENSITY, and the calculated burning rate.

Special topic: Making Fuels Disappear (BURN_AWAY)

If a burning object is to disappear from the calculation once it is consumed, set BURN_AWAY=.TRUE. on the corresponding SURF line. The solid object disappears from the calculation cell by cell, as the mass contained by each mesh cells is consumed either by the pyrolysis reactions or by the prescribed HRR. The mass of each mesh cell is the cell face area multiplied by the surface density of the SURF type.

The following issues should be kept in mind when using BURN_AWAY:

- For reacting surfaces, the surface density is computed as a sum of the layer densities multiplied by the layer thicknesses. This value can be over-ridden by setting SURFACE_DENSITY on the SURF line. For surfaces with prescribed HRR (HRRPUA), SURFACE_DENSITY parameter is the only way of defining the mass of the object.

- Use BURN_AWAY parameter cautiously. If an object has the potential of burning away, a significant amount of extra memory has to be set aside to store additional surface information as the rectangular block is eaten away.

- If BURN_AWAY is prescribed, the SURF should be applied to the entire object, not just a face of the object because it is unclear how to handle edges of solid obstructions that have different SURF_IDs on different faces.

- If the volume of the obstruction changes because it has to conform to the uniform mesh, FDS does **not** adjust the burning rate to account for this as it does with various quantities associated with areas, like HRRPUA.

- A parameter called BULK_DENSITY (kg/m^3) can be applied to the OBST rather than the SURF line. This parameter is used to determine the combustible mass of the solid object. The calculation uses the user-specified object dimensions, not those of the mesh-adjusted object. This parameter over-rides all other parameters from which a combustible mass would be calculated.

- The mass of the object is based on the densities of the all material components (MATL), but it is only consumed by mass fluxes of the **known** species. If the sum of the gaseous yields (Section 11.2.3) is less than one, it will take longer to consume the mass.

Example Case: box_burn_away

This is a silly example of a solid block of "foam" that is pyrolyzed until it is completely consumed. The heat flux is generated by placing hot surfaces around the box. There is no combustion. The properties of the block of foam were chosen simply to assure a quick calculation. The objective of the test is to check that the integrated burning rate is consistent with the material properties of the block. The block is 0.4 m on a side, with a density of 20 kg/m^3. The integrated burning rate (written to box_burn_away_hrr.csv) for a 60 s calculation ought to be:

$$(0.4)^3 \text{ m}^3 \times 20 \text{ kg/m}^3 = 1.28 \text{ kg} \tag{8.9}$$

8.4   Testing Your Pyrolysis Model

Real materials that can burn can be very complicated. Undoubtedly, the `SURF` and `MATL` lines in the input file will consist of a combination of empirical and fundamental properties, often originating from different sources. How do you know that the various property values and the associated thermo-physical model in FDS constitute an appropriate description of the solid? For a full-scale simulation, it is hard to untangle the uncertainties associated with the gas and solid phase routines. However, it is easy to perform a simple check of any set of surface properties by essentially turning off the gas phase – no combustion and no convective heat transfer. There are several parameters that allow you do this, spread out over the various namelist groups.

1. Create a trivially small mesh, just to let FDS run. Since the gas phase calculation is essentially being shut off, you just need 4 cells in each direction (`IJK=4,4,4`) for the pressure solver to function properly.

2. On the `TIME` line, set `WALL_INCREMENT=1` to force FDS to update the solid phase every time step (normally it does this every other time step), and set `DT` to whatever value appropriate for the solid phase calculation. Since there is no gas phase calculation that will limit the time step, it is best to control this yourself.

3. Put `H_FIXED=0.` on the `MISC` line. This turns off the convective heat flux from gas to surface and vis verse. The heat flux to the solid is specified via `EXTERNAL_FLUX` (kW/m^2) on the `SURF` line that is assigned to the solid surface. If you want to specify a particular convective heat flux to the solid surface, you can set `ASSUMED_GAS_TEMPERATURE` on the `MISC` line, along with a non-zero value of `H_FIXED` in units of W/m^2/K.

4. Turn off all the gas phase computations by setting `SOLID_PHASE_ONLY=.TRUE.` on the `MISC` line. This will also speed up the computations significantly. If the gas phase computations are needed, you may turn off combustion by creating a `REAC` line with only `Y_O2_INFTY=0.01`. This sets the background oxygen mass fraction to 0.01, too low to support any burning.

5. Generate `MATL` lines, plus a single `SURF` line, as you normally would, except add `EXTERNAL_FLUX` to the `SURF` line. This is simply a "virtual" source that heats the solid. Think of this as a perfect radiant panel or cone calorimeter.

6. Assign the `SURF_ID` to a `VENT` that spans the bottom of the computational domain. Create `OPEN` vents on all other faces.

7. Finally, add solid phase output devices to the solid surface, like `'WALL TEMPERATURE'`, `'NET HEAT FLUX'`, `'BURNING RATE'`, `'GAUGE HEAT FLUX'`, and `'WALL THICKNESS'` (assuming the solid is to burn away). Use these to track the condition of the solid as a function of time. In particular, make sure that the `'BURNING RATE'` is appropriate for the particular external heat flux applied. Make sure that the `'WALL TEMPERATURE'` is appropriate. Compare your results to measurements made in a bench-scale device, like the cone calorimeter. Keep in mind, however, that the calculation and the experiment are not necessarily perfectly matched. The calculation is designed to eliminate uncertainties related to convection, combustion, and apparatus-specific phenomena.

Example Case: thermoplastic

The term "thermoplastic" is often used to describe materials that essentially heat up and gasify without leaving any solid residue. The term is used here merely to indicate the class of materials for which the pyrolysis can be modeled with a single reaction that converts solid to gaseous fuel.

The purpose of this example is to demonstrate how the solid phase pyrolysis model works in FDS. Essentially, the gas phase calculation is shut off except for the imposition of a 50 kW/m^2 "external" heat flux. The solid in this example is a slab of plastic, similar in composition to PMMA. The solid is described by the following SURF line:

```
&SURF ID='PMMA SLAB'
      COLOR='BLACK'
      MATL_ID='PMMA'
      THICKNESS=0.025
      EXTERNAL_FLUX=50. /  External Flux is ONLY for this simple demo exercise
```

The COLOR is meaningless except to distinguish it in Smokeview. The EXTERNAL_FLUX is a virtual heat source that is only used for these types of diagnostic exercises. The properties of the material are conveyed via the MATL line:

```
&MATL ID='PMMA'
      CONDUCTIVITY=0.21
      SPECIFIC_HEAT=1.5
      DENSITY=1190.
      N_REACTIONS=1
      NU_FUEL=1.
      HEAT_OF_REACTION=1500.
      HEAT_OF_COMBUSTION=25000.
      REFERENCE_TEMPERATURE=330. /
```

Notice that in addition to k, ρ and c, there is one reaction specified, the *yield* of which is 100 % fuel gas (NU_FUEL=1.). The phase change from solid to gas *consumes* energy at a rate of 1,500 kJ/kg. Although not relevant in this example, the burning of these fuel gases would *produce* energy at a rate of 25,000 kJ/kg. The reaction nominally takes place at 330 °C, a necessary parameter for the pyrolysis model described above.

The plots shown in Fig. 8.5 contain the results of the FDS simulation along with what is referred to as "simple theory." By this, we mean that if all of the external heat flux were used to raise the solid temperature to 330 °C and then convert the solid to fuel gas, the results would be as shown by the "simple theory." Of course, the simple theory neglects heat losses through the solid and losses via radiation from the surface. Because it neglects these losses, the simple theory should be regarded as producing an upper bound on the burning rate. Note that the small discontinuities in the FDS burning rate and temperature curves are numerical rather than physical.

Because there is no solid residue produced by the single reaction, the sample thickness will gradually decrease to zero. Note that this does not necessarily mean that the solid obstruction should disappear entirely from the computational domain, but rather that the fuel should be consumed. The parameter BURN_AWAY is used to indicate that the solid ought to be completely removed, but because in this simple test case the sample is aligned with the external boundary of the computational domain, the parameter BURN_AWAY would have no effect. The slab is originally 0.025 m thick, with a density of 1190 kg/m^3. This means there is 29.75 kg/m^2 of fuel present, which if divided by the burning rate (about 0.018 kg/m^2/s) yields a burning time of about 1700 s. After this, the fuel is consumed.
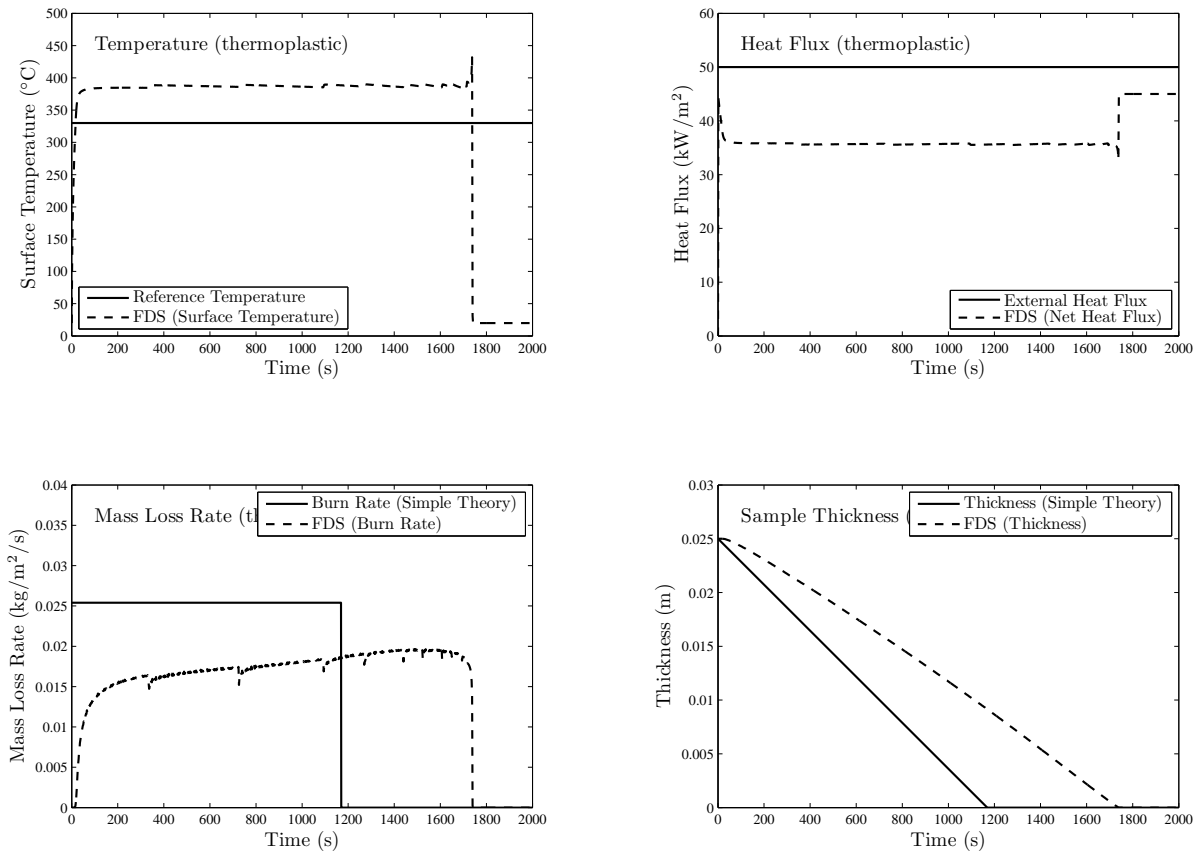
Figure 8.5: Output of **thermoplastic** test case.

Example Case: charring_solid

This example just uses the solid phase algorithm. Essentially, the gas phase is shut off except for the imposition of a 50 kW/m² "external" heat flux. The reaction mechanism is fairly complicated, as it includes various solids like cellulose, char, and water. The sample itself is described via a single SURF line:

```
&SURF ID='SPRUCE'
     STRETCH_FACTOR = 1.
     CELL_SIZE_FACTOR = 0.5
     MATL_ID(1,1:3) = 'CELLULOSE','WATER','LIGNIN'
     MATL_MASS_FRACTION(1,1:3) = 0.70,0.1,0.20
     MATL_ID(2,1) = 'CASI'
     THICKNESS(1:2)  =  0.01,0.01
     EXTERNAL_FLUX = 50. /
```

The sample consists of two layers. The first is a combination of cellulose, water and lignin. There are MATL lines for each. Both cellulose and water have reaction parameters. Cellulose undergoes an endothermic reaction to form an "active" solid, and water evaporates. Lignin does not change form, at least not in this model. The second layer of the sample is a non-reacting slab of calcium silicate board. Note the two parameters on the SURF line called STRETCH_FACTOR and CELL_SIZE_FACTOR. The former tells FDS not to stretch the solid phase nodes used to solve the heat conduction equation. The latter tells FDS to use

cells half the size of what it would use by default, based on the thermal properties. The intent of these two parameters is to increase the spatial resolution of the solid phase mesh to increase the accuracy of the calculation. These kinds of parameters are typically not specified by the user, but a sensitivity analysis might indicate that they ought to be, especially when the reaction sequence is complicated as it is here.

Upon conversion of the virgin cellulose to its "active" component, this latter solid material undergoes two reactions that occur at two different temperatures. The following MATL line describes what is to happen:

```
&MATL ID                  = 'ACTIVE'
      EMISSIVITY          = 1.0
      CONDUCTIVITY_RAMP   = 'k_cell'
      SPECIFIC_HEAT       = 2.3
      DENSITY             = 400.
      N_REACTIONS         = 2
      A(1:2)              = 1.3E10,  3.23E14
      E(1:2)              = 1.505E5, 1.965E5
      HEAT_OF_REACTION(1:2) = 418.,    418.
      NU_RESIDUE(1:2)     = 0.35,    0.0
      NU_FUEL(1:2)        = 0.65,    1.0
      RESIDUE(1)          = 'CHAR' /
```

Notice that the reaction parameters are arrays containing the appropriate information for each reaction, referred to by the numbers 1 and 2. The first reaction converts 35 % (by mass) of the "active" solid to char, and 65 % to fuel gases. The second reaction converts all the mass to fuel gases.

Figure 8.6 shows the surface temperature and burning rate of the sample under the 50 kW/m^2 external heat flux. The burning rate peaks at the start of the simulation, decreases throughout the burning phase, and then increases again at the end due to presence of an external backing material. The initial peak is typical of char-forming solids.
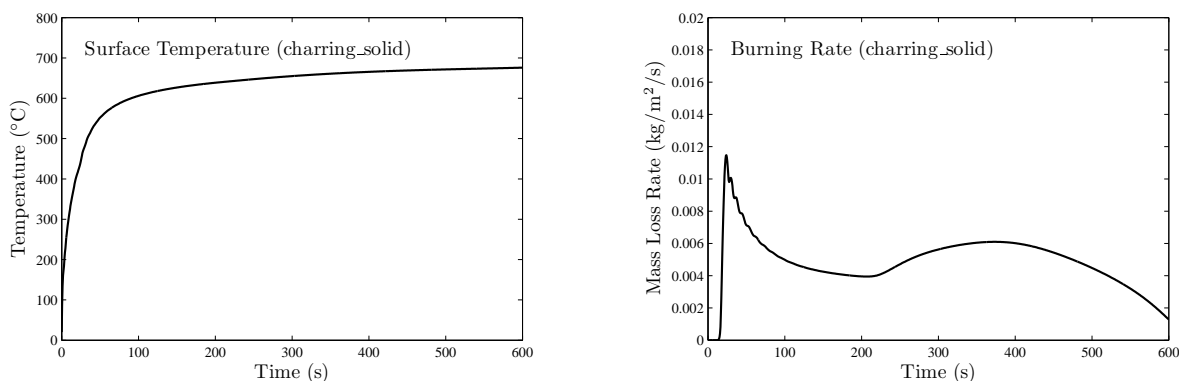
Figure 8.6: Output of **charring_solid** test case.

Example Case: couch and room_fire

In residential fires, upholstered furniture makes up a significant fraction of the combustible load. A single couch can generate several megawatts of energy and sometimes lead to compartment flashover. Modeling a couch fire requires a simplification of its structure and materials. At the very least, we want the upholstery to be described as fabric covering foam:

```
&MATL ID                    = 'FABRIC'
      FYI                   = 'Properties completely fabricated'
      SPECIFIC_HEAT         = 1.0
      CONDUCTIVITY          = 0.1
      DENSITY               = 100.0
      N_REACTIONS           = 1
      NU_FUEL               = 1.
      REFERENCE_TEMPERATURE = 350.
      HEAT_OF_REACTION      = 3000.
      HEAT_OF_COMBUSTION    = 15000. /

&MATL ID                    = 'FOAM'
      FYI                   = 'Properties completely fabricated'
      SPECIFIC_HEAT         = 1.0
      CONDUCTIVITY          = 0.05
      DENSITY               = 40.0
      N_REACTIONS           = 1
      NU_FUEL               = 1.
      REFERENCE_TEMPERATURE = 350.
      HEAT_OF_REACTION      = 1500.
      HEAT_OF_COMBUSTION    = 30000. /

&SURF ID              = 'UPHOLSTERY'
      FYI             = 'Properties completely fabricated'
      COLOR           = 'PURPLE'
      BURN_AWAY       = .TRUE.
      MATL_ID(1:2,1)  = 'FABRIC','FOAM'
      THICKNESS(1:2)  = 0.002,0.1
      PART_ID         = 'smoke' /
```

Both the fabric and the foam decompose into fuel gases via single-step reactions. The fuel gases from each have different composition and heats of combustion. FDS automatically adjusts the mass loss rate of each so that the "effective" fuel gas is that specified by the user on the REAC line. The attribute BURN_AWAY forces FDS to break up the couch into individual cell-sized blocks that will disappear from the calculation as soon as the fuel is exhausted. The surface is specified as consisting of two layers, with a thickness of 2 mm for the FABRIC and 10 cm for the FOAM. The 10 cm is chosen to be the same as the mesh cell size.

The same couch model is included in a room-scale fire simulation, known as the **room_fire** test case. Figure 8.7 shows the fire after 5 and 10 minutes, respectively. Note that after 5 minutes, the couch is fully-involved, and after 10 minutes the room has flashed over. Only the reaction zone of the fire is shown; the smoke is hidden so that you can see the fire progressing from the couch to the doorway at the right of the scene. This door is the only opening to the compartment, and after 10 minutes, the flames can be seen flowing out.
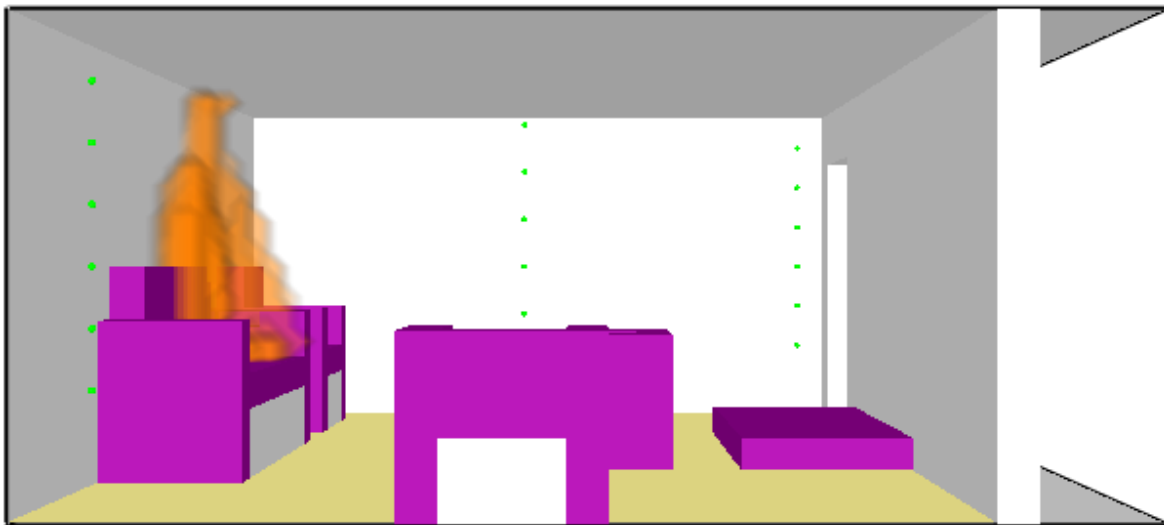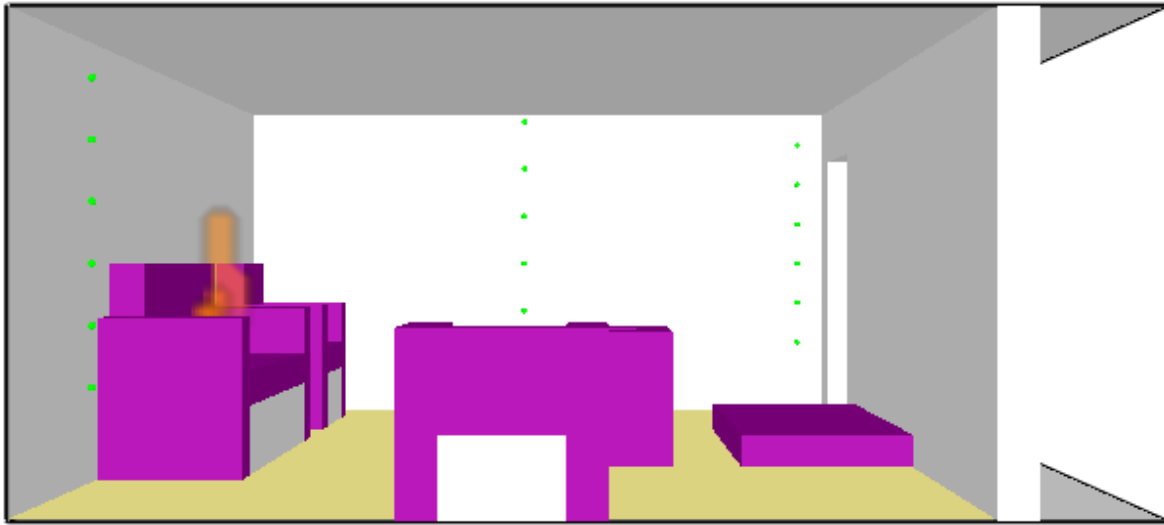
Figure 8.7: Output of **room_fire** test case showing fire after 5 and 10 minutes, respectively.

Example Case: cable_tray

A common combustible in industrial settings are power, control, and instrument cables. The cables may be bundled in a variety of conduits; the most common of which is a ladder-like "tray." From the point of view of FDS, the pile of cables in a tray is a composite of a variety of plastics, insulators, and metal, usually copper. Here is one way to describe a tray of cables:

```
&MATL ID                   = 'PLASTIC'
      CONDUCTIVITY         = 0.2
      SPECIFIC_HEAT        = 1.5
      DENSITY              = 1500.
      N_REACTIONS          = 1
      HEAT_OF_REACTION     = 3000.
      HEAT_OF_COMBUSTION   = 25000.
      REFERENCE_TEMPERATURE = 400.
      NU_FUEL              = 1.0 /

&MATL ID           = 'COPPER'
      SPECIFIC_HEAT = 0.38
      CONDUCTIVITY  = 387.
      DENSITY       = 8940.   /

&SURF ID                     = 'Loose Cable'
      COLOR                  = 'IVORY BLACK'
      MATL_ID(1,1:2)         = 'PLASTIC','COPPER'
      MATL_MASS_FRACTION(1,1:2) = 0.4,0.6
      BACKING                = 'EXPOSED'
      THICKNESS              = 0.02 /

&OBST XB=-2.00, 2.00,-0.14, 0.14, 0.51, 0.55, SURF_ID='Loose Cable' /

&OBST XB=-2.00, 2.00,-0.15,-0.15, 0.50, 0.60, SURF_ID='SHEET METAL' / Tray Side
&OBST XB=-2.00, 2.00, 0.15, 0.15, 0.50, 0.60, SURF_ID='SHEET METAL' / Tray Side
&OBST XB=-1.95,-1.90,-0.15, 0.15, 0.50, 0.50, SURF_ID='SHEET METAL' / Rung
&OBST XB=-1.60,-1.55,-0.15, 0.15, 0.50, 0.50, SURF_ID='SHEET METAL' / Rung
...
&OBST XB= 1.90, 1.95,-0.15, 0.15, 0.50, 0.50, SURF_ID='SHEET METAL' / Rung
```

The pile of cables is assumed to be a solid slab, 28 cm wide and 2 cm deep. The tray is slightly wider and deeper, and because it is listed second in the input file, its surface properties take precedence wherever the cable slab and tray coincide. The mesh cells in this example are 5 cm on a side, but the heat transfer within the cable slab are governed by the 2 cm THICKNESS. The slab is 60 % copper, by mass. Note that we are not assuming multiple layers in this example – the slab is a single layer composite of plastic and copper. The plastic burns at about 400 °, but the copper remains. Thus, the cable does not "burn away."

The point of this test case is merely to propose a simple model of flame spread along a tray of assorted cable. Detailed thermo-physical property data for industrial-grade cable is usually not available, and even if it were, it would probably not improve upon the given model. The properties given in this example are almost completely fabricated. What is important here are the HEAT_OF_REACTION and REFERENCE_TEMPERATURE, obtained in most cases by a bench-scale measurement device like the cone calorimeter.

Chapter 9

Ventilation

This chapter mainly describes how to specify velocity boundary conditions. For fire applications, this is essentially how a ventilation system is modeled.

9.1 Simple Vents, Fans and Heaters

For most applications, the ventilation system of a building is described in FDS using velocity *boundary conditions*. For example, fresh air can be blown into, and smoke can be drawn from, a compartment by specifying a velocity in the *normal* direction to a solid surface. However, there are various other facets of velocity boundary conditions that are described below.

9.1.1 Supply and Exhaust Vents

The easiest way to describe a supply or exhaust fan is to create a `VENT` positioned on a solid surface with a `SURF_ID` with some form of specified velocity or volume flow rate. The normal component of velocity is usually specified directly via the parameter `VEL`. If `VEL` is negative, the flow is directed *into* the computational domain, *i.e.*, a supply vent. If `VEL` is positive, the flow is drawn *out of* the domain, *i.e.*, an exhaust vent. For example, the lines

```
&SURF ID='SUPPLY', VEL=-1.2, COLOR='BLUE' /
&VENT XB=5.0,5.0,1.0,1.4,2.0,2.4, SURF_ID='SUPPLY' /
```

create a `VENT` that *supplies* air at a velocity of 1.2 m/s through an area of nominally 0.16 m^2, depending on the realignment of the `VENT` onto the FDS mesh. Regardless of the orientation of the plane $x = 5$, the flow will be directed *into* the room because of the sign of `VEL`. In this example the `VENT` may not be exactly 0.16 m^2 in area because it may not align exactly with the computational mesh. If this is the case then `VOLUME_FLUX` can be prescribed instead of `VEL`. The units are m^3/s. If the flow is entering the computational domain, `VOLUME_FLUX` should be a negative number, the same convention as for `VEL`. Note that a `SURF` with a `VOLUME_FLUX` prescribed can be invoked by either a `VENT` or an `OBST`, but be aware that in the latter case, the resulting velocity on the face or faces of the obstruction will be given by the specified `VOLUME_FLUX` divided by the area of that particular face. For example:

```
&SURF ID='SUPPLY', VOLUME_FLUX=-5.0, COLOR='GREEN' /
&OBST XB=..., SURF_ID6='BRICK','SUPPLY','BRICK','BRICK','BRICK','BRICK' /
```

dictates that the forward *x*-facing surface of the obstruction is to have a velocity equal to 5 m^3/s divided by the area of the face (as approximated within FDS) flowing into the computational domain.

Note that either `VEL` or `VOLUME_FLUX` should be prescribed, not both. The choice depends on whether an exact velocity is desired at a given vent, or whether the given volume flux is desired.

9.1.2 Heaters

You can create a simple heating vent by changing the temperature of the incoming air

```
&SURF ID='BLOWER', VEL=-1.2, TMP_FRONT=50. /
```

The `VENT` with `SURF_ID='BLOWER'` would blow 50 °C air at 1.2 m/s into the flow domain. Making `VEL` positive would suck air out, in which case `TMP_FRONT` would not be necessary.

Note that if `HRRPUA` or solid phase reaction parameters are specified, no velocity should be prescribed. The combustible gases are ejected at a velocity computed by FDS.

9.1.3 Total Mass Flux

Most often, you specify a simple supply or exhaust vent by setting either a normal velocity or volume flux at a solid surface. However, you may wish to control the mass flow rate (kg/s), as opposed to the volume flow rate (m³/s), via the parameter `MASS_FLUX_TOTAL`. `MASS_FLUX_TOTAL` uses the same sign convention as `VEL` above. In fact, the value entered for `MASS_FLUX_TOTAL` is converted internally into a velocity boundary condition whose value for an outflow is adjusted based on the local density.

9.1.4 Louvered Vents

Most real supply vents are covered with some sort of grill or louvers which act to redirect, or *diffuse*, the incoming air stream. It is possible to mimic this effect, to some extent, by prescribing both a normal and the tangential components of the flow. The normal component is specified with `VEL` as described above. The tangential is prescribed via a pair of real numbers `VEL_T` representing the desired tangential velocity components in the other two coordinate directions (*x* or *y* should precede *y* or *z*). For example, the line

```
&SURF ID='LOUVER', VEL=-1.2, VEL_T=0.5,-0.3 /
```

is a boundary condition for a louvered vent that pushes air into the space with a normal velocity of 1.2 m/s and a tangential velocity of 0.5 m/s in either the *x* or *y* direction and -0.3 m/s in either the *y* or *z* direction, depending on what the normal direction is.

   In cases of limited mesh resolution, it may not be possible to describe a louvered vent or slot diffuser using `VEL_T` because there may not be enough mesh cells spanning the opening. In these cases, you might consider simply specifying a flat plate obstruction in front of the `VENT` with an offset of one mesh cell. The plate will simply redirect the air flow in all lateral directions.

9.1.5 Jet Fans

Fans do not have to be mounted on a solid wall, like a supply or an exhaust fan. If you just want to blow gases in a particular direction, create a thin (zero cells thick) `OBST`ruction and apply to it, via `SURF_ID` only, a `SURF` line that has the parameter `POROUS=.TRUE.` along with the other velocity parameters described above. This allows hot, smokey gases to pass through the obstruction, much like a free-standing fan. These obstructions are merely flat plates, by necessity. The velocity `VEL` associated with a `POROUS` surface is

meant to represent the velocity in the positive or negative coordinate direction, as indicated by its sign. **This is different than the convention used when the** `SURF` **is attached to a solid wall**.

You may also want to construct a *shroud* around the fan using four flat plates arranged to form a short passageway that draws gases in one side and expels them out the other. The plate representing the fan itself can be positioned about halfway along the passage.

A `SURF` with `POROUS=.TRUE.` can only be applied to an `OBST`ruction. It has no meaning when applied to a `VENT`.

9.2 Species and Species Mass Flux Boundary Conditions

There are two species boundary conditions that can be specified (see Section 11.2 for details on inputting and using species). These boundary conditions are `MASS_FLUX(N)` and `MASS_FRACTION(N)` where `N` refers to a given species is via its place in the input file. For example, the second listed species is `N=2`. If a simple no-flux condition is desired at a solid wall, do not set anything. If the mass fraction of the `N`th species is to be some value at a forced flow boundary (`VEL` or `MASS_FLUX_TOTAL`) set `MASS_FRACTION(N)` equal to the desired mass fraction on the appropriate `SURF` line. If the mass flux of the `N`th species is desired, set `MASS_FLUX(N)` instead of `MASS_FRACTION(N)`. If `MASS_FLUX(N)` is set, no `VEL` should be set. It is automatically calculated based on the mass flux. The inputs `MASS_FLUX(N)` (and typically `MASS_FRACTION(N)`) should only be used for inflow boundary conditions. `MASS_FLUX(N)` should be positive with units of kg/m^2/s.

Note that specifying `MASS_FRACTION(N)`, sets the "ghost" cell values for the species mass fractions. Since the mass conservation equation is an advection-diffusion equation, if the specified velocity is small, then the diffusion term can dominate resulting in an unintended mass flux of species. To obtain a guaranteed mass flux of a species, you should use `MASS_FLUX(N)`

9.3 Special Topic: Pressure Boundary Conditions

In some situations, it is more convenient to specify a pressure, rather than a velocity, at a boundary. Suppose, for example, that you are modeling the interior of a tunnel, and a wind is blowing at one of the portals that affects the overall flow within the tunnel. If (and only if) the portal is defined using an `OPEN` vent, then the *dynamic pressure* at the boundary can be specified like this:

```
&VENT XB=..., SURF_ID='OPEN', DYNAMIC_PRESSURE=2.4, PRESSURE_RAMP='wind' /
&RAMP ID='wind', T= 0.0, F=1.0 /
&RAMP ID='wind', T=30.0, F=0.5 /
          .
          .
```

The use of a *dynamic pressure* boundary affects the FDS algorithm as follows. At `OPEN` boundaries, the hydrodynamic pressure (head) $\mathcal{H}$ is specified as

$$\begin{aligned} \mathcal{H} &= \texttt{DYNAMIC\_PRESSURE}/\rho_\infty + |\mathbf{u}|^2/2 \quad \text{(outgoing)} \\ \mathcal{H} &= \texttt{DYNAMIC\_PRESSURE}/\rho_\infty \quad \text{(incoming)} \end{aligned}$$ (9.1)

where ρ_∞ is the ambient density and $\mathbf{u}$ is the most recent value of the velocity on the boundary. The `PRESSURE_RAMP` allows you to alter the pressure as a function of time. Note that you do not need to ramp

the pressure up or down starting at zero, like you do for various other ramps. The net effect of a positive dynamic pressure at an otherwise quiescent boundary is to drive a flow into the domain. However, a fire-driven flow of sufficient strength can push back against this incoming flow.

Example Case: pressure_boundary

The following lines, taken from the sample case, **pressure_boundary**, demonstrates how to do a time-dependent pressure boundary at the end of a tunnel. The tunnel is 10 m long, 1 m wide, 1 m tall with a fire in the middle and a pressure boundary imposed on the right side. The left side (XMIN) is just an OPEN boundary with no pressure specified. It is assumed to be at ambient pressure.

```
&VENT MB = 'XMIN' SURF_ID = 'OPEN' /
&VENT MB = 'XMAX' SURF_ID = 'OPEN', DYNAMIC_PRESSURE=2.4, PRESSURE_RAMP='wind_ramp' /
&RAMP ID='wind_ramp', T= 0., F= 1. /
&RAMP ID='wind_ramp', T=15., F= 1. /
&RAMP ID='wind_ramp', T=16., F=-1. /
```

Figure 9.1 shows two snapshots from Smokeview taken before and after the time when the positive pressure is imposed at the right portal of a tunnel. The fire leans to the left because of the preferential flow in that direction. It leans back to the right when the positive pressure is directed to become negative.
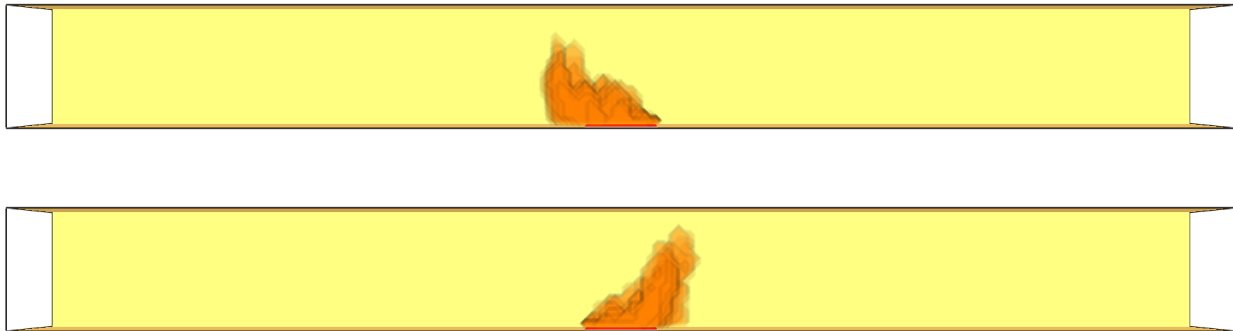
Figure 9.1: Snapshots from the sample case **pressure_boundary** showing a fire in a tunnel leaning left, then right, due to a positive, then negative, pressure imposed at the right portal.

9.4 Special Topic: Fires and Flows in the Outdoors

Simulating a fire in the outdoors is not much different than a fire indoors, but there are a few issues that need to be addressed. First, the velocity of the wind profile at any exterior boundary will be a top hat (constant) by default, but the parameter PROFILE on the SURF line can yield other profiles. For example, PROFILE='PARABOLIC' produces a parabolic profile with VEL being the maximum velocity, and 'ATMOSPHERIC' produces a typical atmospheric wind profile of the form $u = u_0 (z/z_0)^p$. If an atmospheric profile is prescribed, also prescribe Z0 for z_0 and PLE for p. VEL specifies the reference velocity u_0. Note that z_0 is not the ground, but rather some height where the wind speed is measured, like an elevated weather station. It is assumed that the ground is located at $z = 0$. To change this assumption, set GROUND_LEVEL on the MISC line to be the appropriate value of z. Be careful not to apply an atmospheric velocity profile below GROUND_LEVEL or FDS will stop with an error.

Another useful parameter for outdoor simulations is the temperature lapse rate of the atmosphere. Typically, in the first few hundred meters of the atmosphere, the temperature decreases several degrees Celsius per kilometer. These few degrees are important when considering the rise of smoke since the temperature of the smoke decreases rapidly as it rises. The `LAPSE_RATE` of the atmosphere can be specified on the `MISC` line in units of °C/m. A negative sign indicates that the temperature *decreases* with height. This need only be set for outdoor calculations where the height of the domain is tens or hundreds of meters. The default value of the `LAPSE_RATE` is 0 °C/m.

By default, FDS assumes that the density and pressure decrease with height, regardless of the application or domain size. For most simulations, this effect is negligible, but it can be turned off completely by setting `STRATIFICATION=.FALSE.` on the `MISC` line.

9.5 Tangential Velocity Boundary Conditions at Solid Surfaces

As a gas flows past a solid obstruction, it "sticks" to the surface and forms a boundary layer. Ideally, the gas velocity at the surface is zero, and it increases rapidly through a boundary layer that is only a few millimeters thick to its "free-stream" value. In most practical simulations, it is not possible to resolve this boundary layer directly; thus, an empirical model is used to represent its effect on the overall flow field. For a DNS (Direct Numerical Simulation), this discussion is moot. The inner-wall "ghost" cell velocities are set so that the velocity at the wall surface is zero. In other words, the velocity gradient at the wall is computed directly from the resolved velocity vectors near the wall. For an LES (Large Eddy Simulation), the Werner-Wengle wall model is applied. See the FDS Technical Reference Guide [5] for details.

The parameter `SLIP_FACTOR` is no longer used to set the tangential velocity boundary condition, as of FDS version 5.4.0. To force a solid boundary to have a free-slip condition, set `FREE_SLIP=.TRUE.` on the `SURF` line. To force a no-slip boundary condition, set `NO_SLIP=.TRUE.` on the `SURF` line. Otherwise, no parameters need be set – the appropriate wall model will be applied, depending on whether the calculation is a DNS or LES.

9.6 Pressure-Related Effects: The `ZONE` Namelist Group (Table 15.27)

The basic FDS equation set assumes pressure to be composed of a "background" component, $\overline{p}(z,t)$, plus a perturbation, $\tilde{p}(\mathbf{x},t)$. Most often, $\overline{p}$ is just the hydrostatic pressure, and $\tilde{p}$ is the flow-induced pressure field that FDS calculates at each time step. Originally (FDS v. 1-4), it was possible to create a single, sealed compartment whose walls conformed to the exterior of the computational domain. A fire or fan could increase (or decrease) the background pressure in this single compartment, and a leakage area could be defined between the compartment and the ambient exterior. Flow through the "cracks" was simply a function of the background pressure via the usual empirical rules. This idea has been generalized starting in FDS 5. Now, you can specify any number of sealed compartments within the computational domain that can have their own "background" pressures, and these compartments, or "pressure zones," can be connected via leakage and duct paths whose flow rates are tied to the pressure of the adjacent zones.

9.6.1 Specifying Pressure Zones

A pressure zone can by any region within the computational domain that is separated from the rest of the domain, or the exterior, by solid obstructions. There is currently no algorithm within FDS to identify these zones based solely on your specified obstructions. Consequently, it is necessary that you identify these zones explicitly in the input file. The basic syntax for a pressure `ZONE` is:

```
&ZONE XB=0.3,1.2,0.4,2.9,0.3,4.5 /
```

This means that the rectangular region, $0.3 < x < 1.2$, $0.4 < y < 2.9$, $0.3 < z < 4.5$, is assumed to be within a sealed compartment. There can be multiple `ZONE`s declared. The indices of the zones, which are required for the specification of leaks and fans, are determined simply by the order in which they are specified in the input file. By default, the exterior of the computational domain is "Zone 0." If there are no `OPEN` boundaries, the entire computational domain will be assumed to be "Zone 1."

There are several restrictions to assigning pressure zones. First, the declared pressure zones must be completely within a region of the domain that is bordered by solid obstructions. If the sealed region is not rectangular, FDS will extend the specified `ZONE` boundaries to conform to the non-rectangular domain. [1] It is possible to "break" pressure zones by removing obstructions between them.[2] An example of how to break pressure zones is given in Section 9.3. Second, pressure zones **can** span multiple meshes, but it is recommended that you check the pressure in each mesh to ensure consistency. Also, if the `ZONE` does span multiple meshes, make sure that the specified rectangular coordinates do so as well. This allows FDS to determine the actual extent of the `ZONE` independently for each mesh.

Note that if you plan to have one zone open up to another via the removal of an obstruction, make sure that the coordinates of the two zones abut (i.e. touch) even if the one of the zones includes the solid obstruction that separates them. FDS recognizes that a zone boundary has been removed when two adjacent cells belonging to two different zones have no solid obstruction between them. It is recommended that you extend at least one of the zone boundaries *into* the solid obstruction separating the two zones. That way, when the obstruction is removed, the newly created gas phase cells will be assigned to one or the other zone and it will become obvious that two adjacent gas phase cells are of two different zones, at which point the zones will merge and no longer have distinct background pressures.

---

[1] The extension of pressure zones to non-rectangular regions is a feature that started with FDS version 5.3.1.

[2] The ability to open pressure zones became available in FDS starting with version 5.3.0. Prior versions prevented it by issuing an error statement.

9.6.2 Leaks

The volume flow, $\dot{V}$, through a leak of area A_L is given by

$$\dot{V}_{\text{leak}} = A_L \,\text{sign}(\Delta p)\, \sqrt{2\frac{|\Delta p|}{\rho_\infty}} \tag{9.2}$$

where Δp is the pressure difference between the adjacent compartments (in units of Pa) and ρ_∞ is the ambient density (in units of kg/m^3). The discharge coefficient normally seen in this type of formula is assumed to be 1. Leakage is inherently a subgrid-scale phenomenon because the leakage area is usually very small. In other words, it is not possible to define a leak directly on the numerical mesh. It is sometimes possible to "lump" the leaks into a single mesh-resolvable hole, but this is problematic for two reasons. First, the leakage area rarely corresponds neatly to the area of a single mesh cell-sized hole. Second, the flow speeds through the hole can be large and cause numerical instabilities.

A better way to handle leakage is by exploiting pressure zones. A pressure zone is a user-specified volume within the computational domain that is entirely surrounded by solid obstructions. For example, the interior of a closed room can be, and should be, declared a pressure zone. Leakage from one compartment to another is then designated on the input lines defining the individual pressure ZONEs:

```
&ZONE XB=0.3,1.2,0.4,2.9,0.3,4.5, LEAK_AREA(0)=0.0001 /
&ZONE XB=2.3,5.8,1.4,2.9,6.8,9.7, LEAK_AREA(1)=0.0002, LEAK_AREA(0)=0.0003 /
```

The first line designates a region of the computational domain to be "Pressure Zone" 1. Note that the order of the ZONE lines is important; that is, the order implicitly defines Zone 1, Zone 2, *etc.* Zone 0 is by default the ambient pressure exterior. In this example, a leak exists between Zone 1 and the exterior Zone 0, and the area of the leak is 0.0001 m^2 (1 cm by 1 cm hole, for example). Zone 2 leaks to Zone 1 (and vis verse) with a leak area of 0.0002 m^2. Zone 2 also leaks to the outside with an area of 0.0003 m^2. Note that zones need not be connected for a leak to occur. At least one of the obstructions that form the walls of Zone 1 must have the attribute LEAK_PATH=1,0, meaning that the leak between Zones 1 and 0 is uniformly distributed over solids defined with:

```
&SURF ID='whatever',..., LEAK_PATH=1,0 /
```

Likewise, the boundaries of Zone 1 and Zone 2 must include solids whose SURF properties include LEAK_PATH=1,2, but these solids need not form a boundary between the two zones. The SURFaces with the LEAK_PATH attribute lump all of the leakage over these areas. The order of the two pressure zones designated by LEAK_PATH is unimportant.

Example Case: pressure_rise

This example tests several basic features of FDS. A narrow channel, 3 m long, 0.002 m wide, and 1 m tall, has air injected at a rate of 0.1 kg/m^2/s over an area of 0.2 m by 0.002 m for 60 s, with a linear ramp-up and ramp-down over 1 s. The total mass of air in the channel at the start is 0.00718 kg. The total mass of air injected is 0.00244 kg. The domain is assumed two-dimensional, the walls are adiabatic, and STRATIFICATION is set to .FALSE. simply to remove the slight change in pressure and density with height. The domain is divided into three meshes, each 1 m long and each with identical gridding. We expect the pressure, temperature and density to rise during the 60 s injection period. Afterwards, the temperature, density, and pressure should remain constant, according to the equation of state. The figures below show the results of this calculation. The density matches exactly showing that FDS is injecting the appropriate amount of mass. The steady state values of the pressure, density and temperature are consistent with the ideal values.
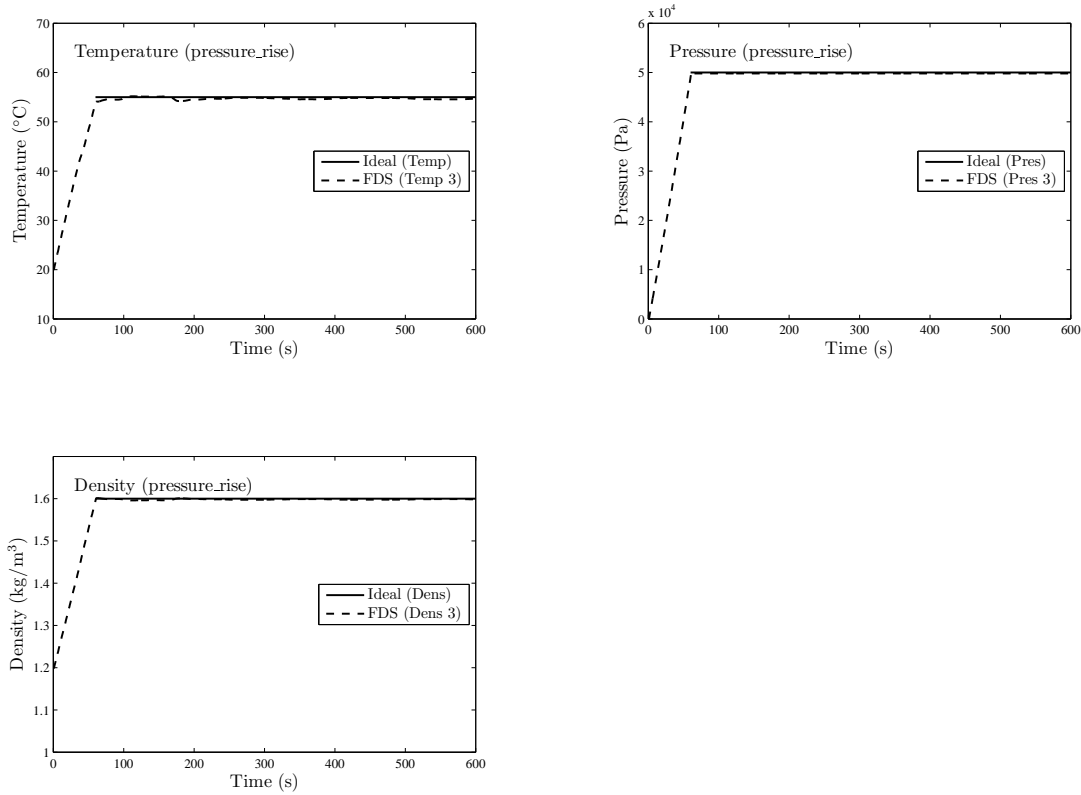
Figure 9.2: Output of **pressure_rise** test case.

Example Case: zone_break

In the example case called **zone_break**, three simple compartments are initially isolated from each other and from the ambient environment outside. Air is blown into compartment 1 at a constant rate for 5 s, increasing its pressure approximately 9500 Pa. At 10 s, compartment 1 is opened to compartment 2, decreasing the overall pressure in the two compartments to roughly one-third the original value because the volume of the combined pressure zone has been roughly tripled. At 15 s, the pressure is further decreased by opening a door to compartment 3, and, finally, at 20 s the pressure returns to ambient following the opening of a door to the outside. Figure 9.3 displays the pressure within each compartment.

Notice that the pressure within each compartment does not come to equilibrium instantaneously. Rather, a relaxation factor is applied by FDS to bring the zones into equilibrium over several seconds. This is done for several reasons. First, in reality doors and windows do not magically disappear as they do in FDS. It takes a finite amount of time to fully open them, and the slowing of the pressure increase/decrease is a simple way to simulate the effect. Second, relatively large pressure differences between zones wreak havoc with flow solvers, especially ones like FDS that use a low Mach number approximation. To maintain numerical stability, FDS gradually brings the pressures into equilibrium. This second point ought to be seen as a warning:

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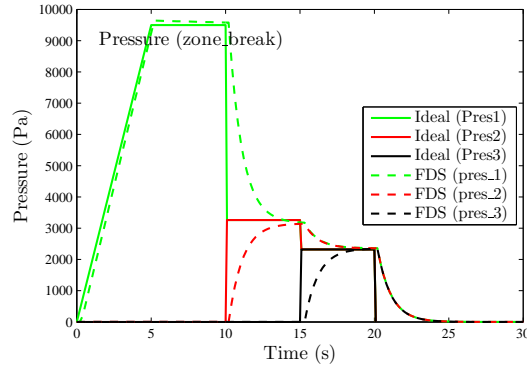
Figure 9.3: Output of **zone_break** test case.

> Do not use FDS to study the sudden rupture of pressure vessels! Its low Mach number formulation does not allow for high speed, compressible effects that are very important in such analyses. The zone breaking functionality described in this example is only intended to be used for relatively small pressure differences (<0.1 atm) between compartments. Real buildings cannot withstand substantially larger pressures anyway.

9.6.3 Fan Curves

In Section 9.1 there is a discussion of velocity boundary conditions, in which a fan is modeled simply as a solid boundary that blows or sucks air, regardless of the surrounding pressure field. In reality, fans operate based on the pressure drop across the duct or manifold in which they are installed. A very simple "fan curve" is given by:

$$\dot{V}_{\text{fan}} = A_{\text{duct}} U_{\text{max}} \, \text{sign}(\Delta p_{\text{max}} - \Delta p) \sqrt{\frac{|\Delta p - \Delta p_{\text{max}}|}{\Delta p_{\text{max}}}} \tag{9.3}$$

The volume flow in the absence of a pressure difference is given by the area of the duct times the velocity of the air. A_{duct} is the area of the duct (m^2), and U_{max} is the air velocity (m/s) in the absence of a pressure difference. The pressure difference, $\Delta p = p_1 - p_2$, indicates the difference in pressure between the downstream compartment, or "zone," and the upstream. The subscript 1 indicates downstream and 2 indicates upstream. The term, Δp_{max}, is the maximum pressure difference the fan can operate upon, and it is assumed to be a positive number. Figure 9.4 displays a typical fan curve.

The velocity of the fan in the absence of a pressure difference, U_{max}, is specified via the parameter VEL on the appropriate SURF line. Alternatively, the volume flow rate, $A_{\text{duct}} U_{\text{max}}$, can be specified using VOLUME_FLUX. Do not use both. These parameters were already introduced in Section 7.1. To simulate the behavior of a real fan, a few extra parameters need to be specified. To set Δp_{max}, the maximum operating over-pressure, add MAX_PRESSURE to the SURF line. Note that MAX_PRESSURE should always be positive and in units of Pa. If the pressure difference (downstream minus upstream) exceeds the specified MAX_PRESSURE, then there will be a backflow in the duct.
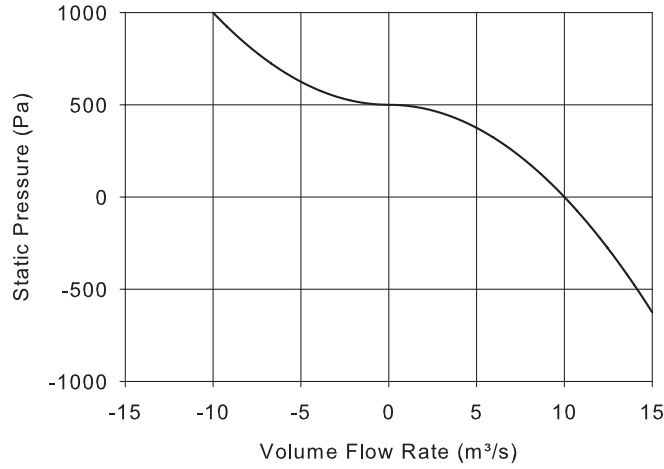
Figure 9.4: Fan curve corresponding to `VOLUME_FLUX=10` and `MAX_PRESSURE=500`. Note that a volume flux greater than 10 is brought about by a negative pressure difference; that is, when the downstream pressure is less than the upstream. Note also that when the pressure difference is greater than 500 Pa, the volume flow becomes negative; that is, the flow reverses.

> Note that the rules governing the sign of `VEL` or `VOLUME_FLUX` remain in force for fans that are subject to pressure differences between compartments. Simply note that the sign of either `VEL` or `VOLUME_FLUX` defines "upstream" and "downstream." Thus, the zone into which air is blown in the absence of a pressure difference is the downstream zone.

Example Case: fan_test

Here is an example how fans can be specified. In it, two simple compartments share a common wall. Both compartments are considered as separate "pressure zones." Two fans are mounted in the Partition Wall, blowing in opposite directions. The relevant input lines are:

```
&SURF ID='BLOW LEFT',  POROUS=.TRUE., VEL=-0.2, DUCT_PATH=1,2, MAX_PRESSURE=1000. /
&SURF ID='BLOW RIGHT', POROUS=.TRUE., VEL= 0.4, DUCT_PATH=2,1, MAX_PRESSURE=1000. /

&ZONE XB=-3.0, 0.0,-1.0, 1.0, 0.0, 2.0 /  Pressure Zone 1
&ZONE XB= 0.0, 3.0,-1.0, 1.0, 0.0, 2.0 /  Pressure Zone 2

&OBST XB= 0.0, 0.0,-1.0, 1.0, 0.0, 2.0 / Partition Wall

&HOLE XB=-0.1, 0.1,-0.1, 0.1, 0.4, 0.6 /
&OBST XB= 0.0, 0.0,-0.1, 0.1, 0.4, 0.6, ..., SURF_ID='BLOW RIGHT', PERMIT_HOLE=.FALSE. /

&HOLE XB=-0.1, 0.1,-0.1, 0.1, 1.4, 1.6 /
&OBST XB= 0.0, 0.0,-0.1, 0.1, 1.4, 1.6, ..., SURF_ID='BLOW LEFT', PERMIT_HOLE=.FALSE. /
```

The volume flow through the fans is given by the expression:

$$\dot{V}_{\text{fan}} = A_{\text{duct}} U_{\text{max}} \, \text{sign}(\Delta p_{\text{max}} - \Delta p) \sqrt{\frac{|\Delta p - \Delta p_{\text{max}}|}{\Delta p_{\text{max}}}} \tag{9.4}$$

where A_{duct} is the area of the duct (both are 0.04 m^2), U_{max} is the air velocity (0.4 m/s from Zone 1 to Zone 2 and 0.2 m/s from Zone 2 to Zone 1), and Δp_{max} is the maximum pressure difference the fan can operate upon (in this case both fans use 1000 Pa).

In steady state, the volume flow from compartment to compartment (or Zone to Zone) should be equal and opposite in sign.

$$(0.04 \text{ m}^2)(0.4 \text{ m/s}) \sqrt{\frac{|p_2 - p_1 - 1000 \text{ Pa}|}{1000 \text{ Pa}}} = (0.04 \text{ m}^2)(0.2 \text{ m/s}) \sqrt{\frac{|p_1 - p_2 - 1000 \text{ Pa}|}{1000 \text{ Pa}}} \quad (9.5)$$

The solution is $p_2 = 300$ Pa and $p_1 = -300$ Pa (see Fig. 9.5). Note that the sign of the Volume Flow in FDS has to do with whether the flow is moving in the plus or minus coordinate direction. This convention can make these types of calculations a bit tricky.
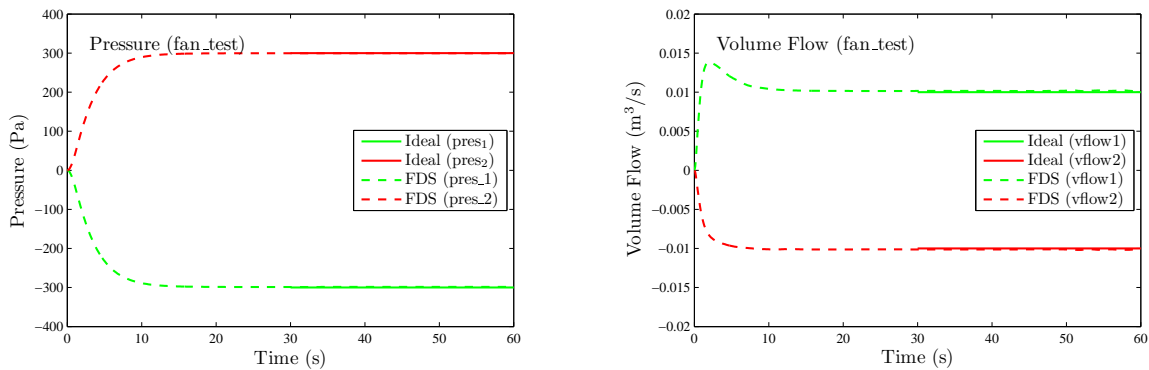
Figure 9.5: Pressure and volume flow for the **fan_test**.

Consider a few of the extra parameters. The attribute `POROUS=.TRUE.` allows hot, smokey gases to pass through the obstructions that represent the fans. These obstructions are merely flat plates, by necessity. The velocity `VEL` associated with a `POROUS` surface is meant to represent the velocity in the positive or negative coordinate direction, as indicated by its sign. This is different than the convention used when the `SURF` is assigned to a solid wall. The `DUCT_PATH` defines the pressure `ZONE`s downstream and upstream of the fan, respectively. The fan represented by the the `SURF` line `ID='BLOW LEFT'`, for example, blows air *into* `ZONE` 1 and draws air *out of* `ZONE` 2 in the absence of a pressure difference between the compartments. The negative value of `VEL` indicates that the fan blows in the negative coordinate direction, into `ZONE` 1 and out of `ZONE` 2, and this is consistent with the order of the `ZONE`s listed by `DUCT_PATH`. In short, `DUCT_PATH` and `VEL` must be coordinated.

The `HOLE`s in the Partition Wall serve only to carve out space for the obstructions that represent the fans. Note the obstructions have zero thickness, as required by the `POROUS` surface. The attribute `PERMIT_HOLE=.FALSE.` tells FDS not to reject the obstructions because they are embedded within the Partition Wall.

Example Cases: leak_test and leak_test_2

In the following examples, both leaks and fans are demonstrated. A simple compartment (3.6 m by 2.4 m by 2.4 m) has a small fan at one end and one leak under the door at the other end. It is assumed for this example that the compartment is contained within a larger compartment that is perfectly sealed. The fan draws air into the compartment from the plenum space, increasing the pressure inside and decreasing it outside. A steady state is achieved when the volume flow into and out of the compartment falls into balance.

The volume flow rate of the fan is given by the "fan curve"

$$\dot{V}_{\text{fan}} = A_{\text{duct}} U_{\text{max}} \, \text{sign}(\Delta p_{\text{max}} - \Delta p) \sqrt{\frac{|\Delta p - \Delta p_{\text{max}}|}{\Delta p_{\text{max}}}} \tag{9.6}$$

where Δp is the difference in pressure and $A_{\text{duct}} = 0.16 \text{ m}^2$, $U_{\text{max}} = 0.1 \text{ m/s}$, and $\Delta p_{\text{max}} = 1000 \text{ Pa}$. The volume flow due to the leak is given by:

$$\dot{V}_{\text{leak}} = A_{\text{leak}} \sqrt{\frac{2\Delta p}{\rho_\infty}} \tag{9.7}$$

where $A_{\text{leak}} = 0.0001 \text{ m}^2$ and $\rho_\infty = 1.2 \text{ kg/m}^3$. After 5 min the pressure difference is 938.2 Pa. The theoretical value, obtained by equating the fan and leak volume flow rates and solving for Δ_p, is 938.9 Pa. The slight difference is due to the fact that the solid boundaries within the interior of the computational domain admit a slight volume flux related to details of the numerical solver.

Just for fun, we add another leak to the compartment, only this time the leak is to the exterior of the entire computational domain, an infinite void at ambient pressure. Now the fan flow rate ought to balance the sum of the flow rates from the two leaks. After 5 min, the pressure difference is 935.2 Pa. The two cases are summarized in Fig. 9.6.
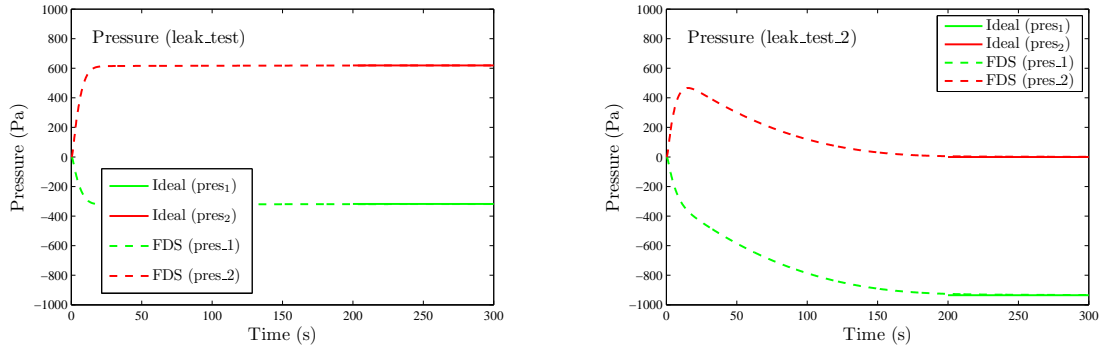
Figure 9.6: Output of the leak test cases.

Chapter 10

User-Specified Functions

Many of the parameters specified in the input file are fixed constants. However, there are several parameters that may vary in time, temperature, or space. These functions can be complex, thus you have to have some way to convey them. The namelist group `RAMP` and `TABL`, as it names imply, allow you to control the behavior of selected parameters. `RAMP` allows you to specify a function with one independent variable (such as time) is mapped to one dependent variable (such as velocity). `TABL` allows for the specification of a mapping from multiple independent variables (such as a solid angle) to multiple dependent variables (such as a sprinkler flow rate and droplet speed).

10.1 Time-Dependent Functions

At the start of any calculation, the temperature is ambient everywhere, the flow velocity is zero everywhere, nothing is burning, and the mass fractions of all species are uniform. When the calculation starts temperatures, velocities, burning rates, *etc.*, are ramped-up from their starting values because nothing can happen instantaneously. By default, everything is ramped-up to their prescribed values in roughly 1 s. However, control the rate at which things turn on, or turn off, by specifying time histories for the boundary conditions that are listed on a given `SURF` line. The above boundary conditions can be made time-dependent using either prescribed functions or user-defined functions. The parameters `TAU_Q`, `TAU_T`, and `TAU_V` indicate that the heat release rate (`HRRPUA`); surface temperature (`TMP_FRONT`); and/or normal velocity (`VEL`, `VOLUME_FLUX`), or `MASS_FLUX_TOTAL` are to ramp up to their prescribed values in `TAU` seconds and remain there. If `TAU_Q` is positive, then the heat release rate ramps up like $\tanh(t/\tau)$. If negative, then the HRR ramps up like $(t/\tau)^2$. If the fire ramps up following a t^2 curve, it remains constant after `TAU_Q` seconds. These rules apply to `TAU_T` and `TAU_V` as well. The default value for all `TAU`s is 1 s. If something other than a tanh or t^2 ramp up is desired, then a user-defined burning history must be input. To do this, set `RAMP_Q`, `RAMP_T` or `RAMP_V` equal to a character string designating the ramp function to use for that particular surface type, then somewhere in the input file generate lines of the form:

```
&RAMP ID='rampname1', T= 0.0, F=0.0 /
&RAMP ID='rampname1', T= 5.0, F=0.5 /
&RAMP ID='rampname1', T=10.0, F=0.7 /
                  .
                  .
                  .
&RAMP ID='rampname2', T= 0.0, F=0.0 /
&RAMP ID='rampname2', T=10.0, F=0.3 /
&RAMP ID='rampname2', T=20.0, F=0.8 /
                  .
```

.
.

Here, `T` is the time, and `F` indicates the fraction of the heat release rate, wall temperature, velocity, mass fraction, *etc.*, to apply. Linear interpolation is used to fill in intermediate time points. Note that each set of `RAMP` lines must have a unique `ID` and that the lines must be listed with monotonically increasing `T`. Note also that the `TAU`s and the `RAMP`s are mutually exclusive. For a given surface quantity, both cannot be prescribed.

As an example, the simple blowing vent from above can be controlled via the lines:

```
&SURF ID='BLOWER',VEL=-1.2,TMP_FRONT=50., RAMP_V='BLOWER RAMP', RAMP_T='HEATER RAMP' /
&RAMP ID='BLOWER RAMP', T= 0.0, F=0.0 /
&RAMP ID='BLOWER RAMP', T=10.0, F=1.0 /
&RAMP ID='BLOWER RAMP', T=80.0, F=1.0 /
&RAMP ID='BLOWER RAMP', T=90.0, F=0.0 /
&RAMP ID='HEATER RAMP', T= 0.0, F=0.0 /
&RAMP ID='HEATER RAMP', T=20.0, F=1.0 /
&RAMP ID='HEATER RAMP', T=30.0, F=1.0 /
&RAMP ID='HEATER RAMP', T=40.0, F=0.0 /
```

Now the temperature and velocity of the incoming air stream would follow the same ramp functions. Note that the temperature and velocity can be independently controlled by assigning different `RAMP`s to `RAMP_T` and `RAMP_V`, respectively.

Use `TAU_T` or `RAMP_T` to control the ramp-ups for surface temperature. The surface temperature will be computed as

$$T_W(t) = \texttt{TAMB} + f(t)\,(\texttt{TMP\_FRONT} - \texttt{TAMB}) \tag{10.1}$$

where $T_W(t)$ is the surface temperature to be applied, $f(t)$ is the result of evaluating the `RAMP_T` at time t, `TAMB` is the input specified on the `MISC` line, and `TMP_FRONT` is the input specified on the `SURF` line that the `RAMP_T` is for.

Use `TAU_MF(N)` or `RAMP_MF(N)` to control the ramp-ups for either the mass fraction or mass flux of species `N`. The mass fraction of species N at the surface is given by

$$Y_N(t) = Y_N(0) + f(t)\,(Y_N - Y_N(0))$$

where $Y_N(0)$ is the ambient mass fraction of species `N` (`MASS_FRACTION_0` in the `N`th `SPEC` namelist line is used to prescribe $Y_N(0)$), Y_N is the desired mass fraction to which the function $f(t)$ is ramping (`MASS_FRACTION(N)` specified in the `SURF` line is used to prescribe Y_N). The function $f(t)$ is either a tanh, t^2, or user-defined function. For a user-defined function, indicate the name of the ramp function with `RAMP_MF(N)`, a character string.

10.2 Temperature-Dependent Functions

Thermal properties like conductivity and specific heat can vary significantly with temperature. In such cases, use the `RAMP` function like this:

```
&MATL ID               = 'STEEL'
      FYI              = 'A242 Steel'
      SPECIFIC_HEAT_RAMP = 'c_steel'
      CONDUCTIVITY_RAMP  = 'k_steel'
      DENSITY          = 7850. /
```

```
&RAMP ID='c_steel', T= 20., F=0.45   /
&RAMP ID='c_steel', T=377., F=0.60   /
&RAMP ID='c_steel', T=677., F=0.85   /

&RAMP ID='k_steel', T= 20., F=48.    /
&RAMP ID='k_steel', T=677., F=30.    /
```

Note that here (as opposed to time ramps) the parameter `F` is the actual physical quantity, not just a fraction of some other quantity. Thus, if `CONDUCTIVITY_RAMP` is used, there should be no value of `CONDUCTIVITY` given. Note also that for values of temperature, `T`, below and above the given range, FDS will assume a constant value equal to the first or last `F` specified.

10.3 Tabular Functions

Some input quantities, such as a sprinkler spray pattern, vary multi-dimensionally. In such cases, use the `TABL` namelist group. The format of the `TABL` lines is application-specific, but in general look like this:

```
&TABL ID='TABLE1', TABLE_DATA=40,50, 85, 95,10,0.5 /
&TABL ID='TABLE1', TABLE_DATA=40,50,185,195,10,0.5 /
```

A detailed description of the various table entries is given in the sections that describe quantities that use such tables. Currently, only sprinklers and nozzles use this group of parameters to define a complex spray pattern.

Note that each set of `TABL` lines must have a unique `ID`. Specific requirements on ordering the lines will depend upon the type of TABL and those requirements are provided in the appropriate section in this guide.

Chapter 11

Combustion and Radiation

A common source of confusion in FDS is the distinction between gas phase *combustion* and solid phase *pyrolysis*. The former refers to the reaction of fuel vapor and oxygen; the latter the generation of fuel vapor at a solid or liquid surface. Whereas there can be many types of combustibles in an FDS fire simulation, there can only be one gaseous fuel. The reason is cost. It is expensive to solve transport equations for multiple gaseous fuels. Consequently, the burning rates of solids and liquids are automatically adjusted by FDS to account for the difference in the heats of combustion of the various combustibles. In effect, you specify a single gas phase reaction as a surrogate for all the potential fuel sources.

The gas phase reaction can be described in two ways. By default, a so-called *mixture fraction* model is used to account for the evolution of the fuel gas from its surface of origin through the combustion process. The alternative is what is referred to as the *finite-rate* approach, where all of the individual gas species involved in the combustion process are defined and tracked individually, and the combustion process is modeled as one or more finite-rate reactions of these species. This is a costlier and more complicated approach than the *mixture fraction* model. This chapter describes both methods, with an emphasis on the more commonly used mixture fraction model.

11.1   Mixture Fraction Combustion: The `REAC` Namelist Group

There are two ways of modeling a fire. The first is to *specify* explicitly a Heat Release Rate Per Unit Area, `HRRPUA`, on a `SURF` line and then apply the `SURF_ID` to an obstruction or vent. This essentially creates a gas burner whose fuel flow rate you explicitly control. The other way to model a fire is to specify solid phase thermal and pyrolysis properties on one or more `MATL` lines, assemble these materials via a `SURF` line, and then apply this boundary condition to obstructions or vents. In this case the burning rate of the fuel depends on the net heat feedback to the surface. In both cases, however, the mixture fraction combustion model is used by default. In fact, the mere presence of these parameters automatically invokes the mixture fraction model[1]. Do not specify explicitly gas species like oxygen if you have also specified the heat release rate per unit area, `HRRPUA`, or solid phase reaction rates.

11.1.1   Basics

The stoichiometry of the gas phase combustion reaction or reactions is specified using the `REAC` namelist group. For the default mixture fraction model, only a single `REAC` line is needed. If the `REAC` line is not found in the input file, propane will be used as the surrogate fuel, and all burning rates will be adjusted accordingly.

---

[1]There is an exception to this rule. It is possible to use the finite-rate combustion model in conjuction with a pyrolysis model that generates the specified gaseous fuel species.

If you only specify the fire's heat release rate with `HRRPUA`, then the reaction parameters may not require adjusting, and no `REAC` line need be added to the input file. However, if you know something about the predominant fuel gas, you might want to consider specifying, at the very least, the basic stoichiometry via the `REAC` line.

Using the mixture fraction model, each reaction is assumed to be of the form:

$$C_xH_yO_zN_vOther_w + \nu_{O_2} O_2 \rightarrow \nu_{CO_2} CO_2 + \nu_{H_2O} H_2O + \nu_{CO} CO + \nu_{soot} Soot + \nu_{N_2} N_2 + \nu_{H_2} H_2 + \nu_{Other} Other \tag{11.1}$$
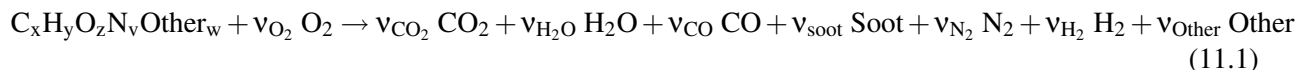
You need only specify the chemical formula of the fuel along with the yields of CO, soot, and H_2, and the amount of hydrogen in the soot, H_{frac}. For completeness you can specify the N_2 content of the fuel and the presence of other species. FDS will use that information internally to determine the amount of combustion products that are formed:

$$
\begin{aligned}
\nu_{O_2} &= \nu_{CO_2} + \frac{\nu_{CO}}{2} + \frac{\nu_{H_2O}}{2} - \frac{z}{2} \\
\nu_{CO_2} &= x - \nu_{CO} - (1 - H_{frac})\nu_{soot} \\
\nu_{H_2O} &= \frac{y}{2} - \frac{H_{frac}}{2}\nu_{soot} - \nu_{H_2} \\
\nu_{CO} &= \frac{W_f}{W_{CO}}y_{CO} \\
\nu_{H_2} &= \frac{W_f}{W_{H_2}}y_{H_2} \\
\nu_{soot} &= \frac{W_f}{W_s}y_s \\
\nu_{N_2} &= \frac{v}{2} \\
\nu_{other} &= w \\
W_s &= H_{frac} W_H + (1 - H_{frac}) W_C
\end{aligned}
$$

The following parameters may be prescribed on the `REAC` line. Note that the various `YIELD`s are for well-ventilated, post-flame conditions. There are options to predict various species yields in under-ventilated fire scenarios, but these special models still require the post-flame yields for CO, soot and any other species listed below.

`ID` A character string that identifies the reaction. Normally, this label is not used by FDS, but it is useful to label the `REAC` line to more easily identify the fuel species.

`C, H, O, N, OTHER` The fuel chemical formula. All numbers are positive. (Mixture Fraction only, default values are those of propane)

`MW_OTHER` Average molecular weight for `OTHER` (g/mol). (Mixture Fraction only, default is the molecular weight of N_2, 28 g/mol)

`Y_O2_INFTY` Ambient mass fraction of oxygen (Mixture Fraction only, default 0.23)

`Y_F_INLET` Mass fraction of fuel in fuel stream (Mixture Fraction only, default 1.0)

`SOOT_YIELD` The fraction of fuel mass converted into smoke particulate, y_s. Note that this parameter does not apply to the processes of soot growth and oxidation, but rather to the net production of the smoke particulate from the fire. (Mixture Fraction only, default 0.01)

SOOT_H_FRACTION The fraction of the atoms in the soot that are hydrogen. (Mixture Fraction only, default 0.1)

CO_YIELD The fraction of fuel mass converted into carbon monoxide, y_{CO}. (Mixture Fraction only, default 0.0)

H2_YIELD The fraction of fuel mass converted into hydrogen, y_{H_2}. (Mixture Fraction only, default 0.0)

HEAT_OF_COMBUSTION ΔH (kJ/kg). The amount of energy released per unit mass of fuel consumed. Note that if the heat of combustion is not specified, it is assumed to be

$$\Delta H \approx \frac{\nu_{O_2} W_{O_2}}{\nu_f W_f} \text{ EPUMO2} \qquad \text{kJ/kg} \tag{11.2}$$

EPUMO2 The amount of energy released per unit mass of oxygen consumed. (kJ/kg) Default is 13,100 kJ/kg. Note that if both EPUMO2 and HEAT_OF_COMBUSTION are specified that FDS will ignore the value for EPUMO2.

IDEAL Logical value indicating whether or not the EPUMO2 or HEAT_OF_COMBUSTION values represent values for complete combustion (.TRUE.) or for incomplete combustion (.FALSE.), i.e. the values account for the specified y_{CO}, y_{H_2}, and y_s. If IDEAL=.TRUE., then FDS will internally adjust ΔH to account for products of incomplete combustion. The default value is .FALSE.

A few sample REAC lines are given here. The values are for demonstration only.

```
&REAC ID           = 'METHANE'
      C            = 1.
      H            = 4. /

&REAC ID                 = 'PROPANE'
      SOOT_YIELD         = 0.01
      C                  = 3.
      H                  = 8.
      HEAT_OF_COMBUSTION = 46460.
      IDEAL              = .TRUE. /

&REAC ID                 = 'PROPANE'
      SOOT_YIELD         = 0.01
      C                  = 3.
      H                  = 8.
      HEAT_OF_COMBUSTION = 46124.
      IDEAL              = .FALSE. /

&REAC ID                 = 'ACRYLONITRILE'
      C                  = 3.
      H                  = 3.
      N                  = 1.
      HEAT_OF_COMBUSTION = 24500.
      IDEAL              = .TRUE. /

&REAC ID                 = 'CARBON DISULFIDE'
      C                  = 1.
      Other              = 2.
      MW_OTHER           = 32.
      HEAT_OF_COMBUSTION = 13600.
      IDEAL              = .TRUE. /
```

11.1.2 Special Topic: Heat of Combustion

By default, the Energy Per Unit Mass of Oxygen, `EPUMO2`, is used to compute the heat of combustion according to Eq. (11.2). Specifying the `HEAT_OF_COMBUSTION` will override this computation. However, if heats of reaction have been specified on the `MATL` line and the heat of combustion of the material differs from that specified by the governing gas phase reaction, then add a `HEAT_OF_COMBUSTION` (kJ/kg) to the `MATL` line. With the mixture fraction combustion model, it is assumed that there is only one fuel. However, in a realistic fire scenario, there may be many fuel gases generated by the various burning objects in the building. Specify the stoichiometry of the predominant reaction via the `REAC` namelist group. If the stoichiometry of the burning material differs from the global reaction, the `HEAT_OF_COMBUSTION` is used to ensure that an equivalent amount of fuel is injected into the flow domain from the burning object.

11.1.3 Special Topic: Flame Extinction

Modeling suppression of a fire due to the introduction of a suppression agent like CO_2 or water mist, or due to the exhaustion of oxygen within a compartment is challenging because the relevant physical mechanisms occur at length scales smaller than a single mesh cell. Flames are extinguished due to lowered temperatures and dilution of the oxygen supply. A simple suppression algorithm has been implemented in FDS that attempts to gauge whether or not a flame is viable at the fuel-oxygen interface. The Technical Reference Guide [1] contains more details about how the mechanism works. The only parameters you can control are the Limiting Oxygen Index, `X_O2_LL`, and the `CRITICAL_FLAME_TEMPERATURE`. Both are set on the `REAC` line. The default values are 0.15 (volume fraction) and 1427 °C, respectively. To eliminate any gas phase suppression, set `X_O2_LL` to 0, or turn off suppression completely by setting `SUPPRESSION=.FALSE.` on the `MISC` line. This latter approach saves on computing time because it prevents FDS from entering the suppression algorithm altogether.

Example Case: door_crack

This example uses the same simple compartment that was used to test leakage and fan curves. Now, we add a small (160 kW) fire, with the same fan and leak under the door. The compartment now opens to the atmosphere, not a sealed plenum. We expect a rapid pressure rise in the compartment due to the effect of the fire and the fan. Initially, the pressure rises due to the heat from the fire and the fan blowing air into the compartment:

$$\frac{d\overline{p}_1}{dt} \approx (\gamma - 1)\frac{\dot{Q}}{V} + \gamma \overline{p}\frac{\dot{V}}{V} \approx 3200 \text{ Pa/s} \approx 0.03 \text{ atm/s} \tag{11.3}$$

where $\gamma \approx 1.4$, $\dot{Q} = 160,000$ W, $V = 20.7$ m^3, and $\dot{V} = 0.016$ m^3/s. However, as heat is lost to the walls, and as the leak begins to relieve the pressure increase, the pressure rise slows, and then reverses at about 0.25 atm. In roughly 150 s, the fire is self-extinguished due to lack of oxygen. As the pressure rise decreases back to zero, and actually goes below zero, the fan, and the leak under the door, increase the oxygen supply, at least near these openings, and the fuel-rich gases in the compartment continue to burn.

While this case has a number of interesting physical effects, and it *verifies* several features of FDS, it is very important to note the following:

- Although there is smoke seen flowing backwards out the fan duct, in reality there would have been much more. Most conventionally built structures will not withstand over-pressures of 0.25 atm without some sort of relief. The fan and the crack under the door obey simple formulae based on pressure differences, but these assumptions have limits.

- It is likely that the fire in this scenario would indeed extinguish itself as the oxygen volume fraction decreased below about 15 %. **But,** its re-ignition at the door crack and fan grill would depend on the
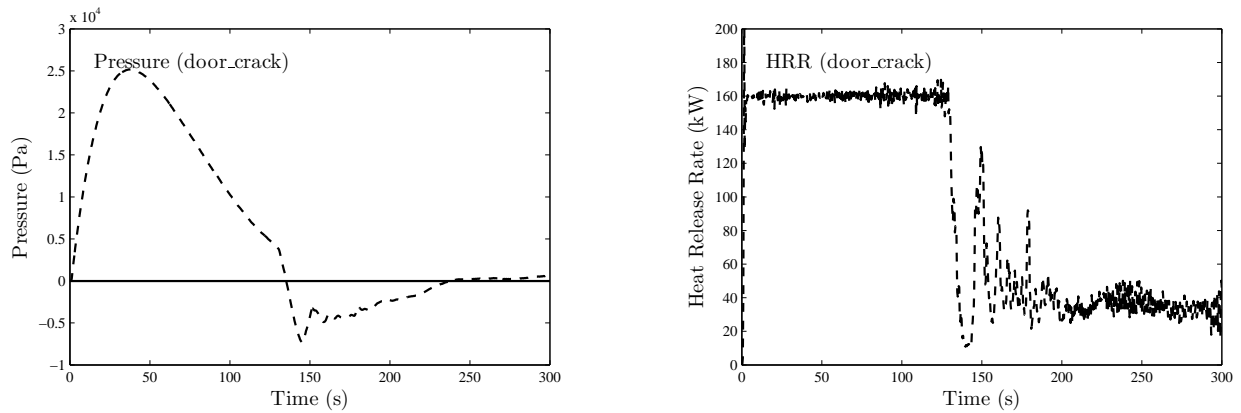
Figure 11.1: Output of **door_crack** test case.

presence of a spark or hot spot of some sort. FDS continues to flow fuel into the compartment past the point of local extinction, but the compartment cools. The default combustion algorithm in FDS assumes that in every grid cell there is a "virtual spark plug" that initiates combustion if fuel and oxygen are present.

11.1.4 Special Topic: CO Production

An algorithm has been implemented that computes the combustion as a two step reaction that predicts the formation and destruction of CO. The Technical Reference Guide [1] contains more details about how the mechanism works. This algorithm is used when CO_PRODUCTION is set to .TRUE. on the MISC line. Even though the algorithm predicts CO formation and its eventual oxidation at elevated temperature, it cannot predict the post-flame yield of CO. For example, within a flashed over compartment, the algorithm predicts the elevated CO levels, but it cannot predict the CO concentration of the exhaust gases that exit the flaming region. Thus, even if using this model, you must specify the CO_YIELD that is expected of a well-ventilated fire.

Note that when active, this algorithm requires the use of three parameters for the mixture fraction compared to the default two and will therefore increase run times and memory usage accordingly. If the simulation you are performing will not result in an under-ventilated fire, then there will be of little if any benefit to enabling the CO production algorithm.

11.1.5 Special Topic: Turbulent Combustion

Unless you are performing a Direct Numerical Simulation (DNS), the reaction rate of fuel and oxygen is not based on the diffusion of fuel and oxygen at a well-resolved flame sheet. Instead, semi-empirical rules are invoked by FDS to determine the rate of mixing of fuel and oxygen within a given mesh cell at a given time step. This section provides a brief explanation of these rules and the parameters that control them.

In an LES simulation, the heat release rate is computed as

$$\dot{q}''' = \frac{\max\left(\rho Y_{\mathrm{F}}, s\rho Y_{\mathrm{O_2}}\right)}{\tau} \Delta H \quad ; \quad s = \frac{W_{\mathrm{F}}}{\nu_{\mathrm{O_2}} W_{\mathrm{O_2}}} \tag{11.4}$$

99

Here, τ is a mixing time scale [6] given by

$$\tau = \frac{C \, (\delta x \, \delta y \, \delta z)^{\frac{2}{3}}}{D_{\mathrm{LES}}} \tag{11.5}$$

The coefficient, C, is taken as 0.1 in FDS by default, based on comparisons to various flame height correlations. It is given by `C_EDC` on the `REAC` line. If you do not want to use this model, set `EDDY_DISSIPATION=.FALSE.` on the `REAC` line, in which case τ becomes the time step, δt.

There are two additional bounds on the local heat release rate per unit volume. One is based on an empirically determined maximum heat release rate per unit area of flame sheet:

$$\dot{q}'''_{\mathrm{max},1} = \frac{\dot{q}''_{\mathrm{max}}}{(\delta x \, \delta y \, \delta z)^{\frac{1}{3}}} \tag{11.6}$$

The parameter $\dot{q}''_{\mathrm{max}}$ is called `HRRPUA_SHEET` on the `REAC` line and its default value is 200 kW/m^2. The second bound is based on an empirical estimate of the average volumetric heat release rate of a fire.

$$\dot{q}'''_{\mathrm{max},2} = \frac{\overline{\dot{q}'''_{\mathrm{max}}} - (1 - \delta t/\tau') \, \overline{\dot{q}'''}}{\delta t/\tau'} \tag{11.7}$$

Orloff and De Ris [7] suggest a value of 1200 kW/m^3, and FDS uses by default a value of 3000 kW/m^3 as an upper bound (`HRRPUV_AVERAGE` on the `REAC` line). Here, τ' is an averaging time that should be larger than the pulsation period of the fire. It is given by `HRRPUV_AVERAGE_TIME` on the `REAC` line. It is 1 s by default.

11.2 Extra Gas Species: The `SPEC` Namelist Group

Normally when you specify a fire via either `HRRPUA` on the `SURF` line or reaction parameters on the `MATL` line, the mixture fraction combustion model is applied. A a set of two or three scalar variables, Z_i, represent the state of the combustion process from pure fuel ($\sum Z_i = 1$) to pure air ($\sum Z_i = 0$). The major reactants and products of combustion – fuel, O_2, CO_2, H_2O, N_2, CO and soot – are all pre-tabulated functions of the mixture fraction, Z. In other words, the values of Z_i in any given mesh cell determines the mass fraction of all the gases listed. The fuel chemistry listed under the `REAC` namelist group is used to generate the table associating the mass fractions with Z_i. You need not, *and should not*, explicitly list the reactants and products of combustion.

Suppose however that gases are introduced into the domain that are neither reactants nor products of combustion. This gas can be tracked separately from the mixture fraction via an additional scalar transport equation[2]. In fact, there does not need to be any fire at all – FDS can be used to transport a mixture of non-reacting ideal gases.

11.2.1 Basics

The namelist group `SPEC` is used to specify each additional gas species. Each `SPEC` line should include at the very least the name of the species via a character string called (`ID`). Next, if the ambient (initial) mass fraction of the gas is something other than 0, then the parameter `MASS_FRACTION_0` is used to specify it. Several gases that can be included in a calculation are listed in Table 11.1. Here is an example:

```
&SPEC ID='ARGON',MASS_FRACTION_0=0.1,MW=40. /
```

Once the extra species has been declared, you introduce it at surfaces via the parameters `MASS_FRACTION(N)` or `MASS_FLUX(N)`. The index `N` refers to the order in which the species is listed in the input file. Following is a very simple example of how a gas can be introduced into the simulation.

Sample Case: gas_filling

Consider the short input file:

```
&HEAD CHID='gas_filling', TITLE='Fill an Empty Room with Hydrogen' /
&MESH IJK=32,32,15, XB=-3.2,3.2,-3.2,3.2,0.0,3.0 /
&TIME T_END=300.0 /
&SPEC ID='HYDROGEN' /
&SURF ID='LEAK', MASS_FLUX(1)=0.01667, RAMP_MF(1)='leak_ramp' /
&RAMP ID='leak_ramp', T=  0., F=0.0 /
&RAMP ID='leak_ramp', T=  1., F=1.0 /
&RAMP ID='leak_ramp', T=180., F=1.0 /
&RAMP ID='leak_ramp', T=181., F=0.0 /
&VENT XB=-0.6,0.4,-0.6,0.4,0.0,0.0, SURF_ID='LEAK', COLOR='RED' /
&DUMP MASS_FILE=.TRUE. /
&SLCF PBY=0.0, QUANTITY='HYDROGEN' /
&TAIL /
```

The case is nothing more than hydrogen gas filling a box. The gas is injected through a 1 m by 1 m vent at a rate of 0.01667 kg/m²/s and shut off after 3 m. The total mass of hydrogen at that point ought to be 3 kg (see

---

[2] Often an extra gas introduced into a calculation is the same as a product of combustion, like water vapor from a sprinkler or carbon dioxide from an extinguisher. These gases are tracked separately, thus water vapor generated by the combustion is tracked via the mixture fraction variable and water vapor generated by evaporating sprinkler droplets is tracked via its own transport equation. In the case of sprinklers, do not specify `'WATER VAPOR'` as an extra species – it is done automatically.

Fig. 11.2). Notice that no properties were needed for the HYDROGEN because it is a species whose properties have already been programmed into FDS. The background species in this case is assumed to be air. The mass flow rate of the hydrogen is controlled via the ramping parameter RAMP_MF(1), and the index 1 refers to the first, and only, gas species that is specified in the input file. The parameter MASS_FILE=.TRUE. instructs FDS to produce an output file that contains a time history of the hydrogen mass.
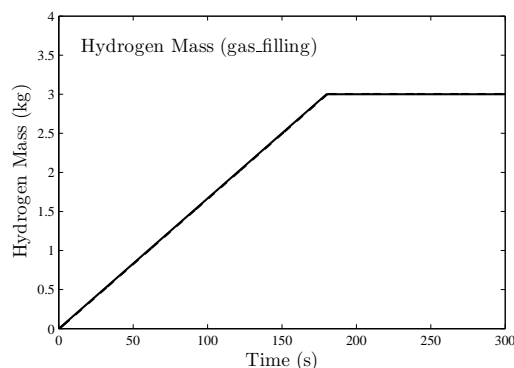
Figure 11.2: Hydrogen mass vs. time for **gas_filling** test case.

11.2.2 Special Topic: Gas Species Properties

Gases whose properties are hardwired in FDS are listed in Table 11.1. The physical properties of these gases are known and do not need to be specified. However, if a desired gas is not included in Table 11.1, its molecular weight MW must be specified on the SPEC line in units of g/mol. In addition, if a DNS calculation is being performed, either the Lennard-Jones potential parameters σ (SIGMALJ) and ε/k (EPSILONKLJ) should be specified; or the VISCOSITY (kg/m/s), CONDUCTIVITY (W/m/K), and DIFFUSIVITY (m^2/s) between the given species and the background species should be specified.

If the simulation does not involve the mixture fraction model – either because no combustion is desired or if a finite rate reaction(s) is being specified (see Section 11.2.4) – you can specify that the background gas species be something other than air. For a gas mixture comprised of n species, FDS only solves transport equations for $n-1$ because it also solves an equation for total mass conservation. To set the properties of the implicitly defined BACKGROUND_SPECIES, use the MISC line. If this species is not listed in Table 11.1, specify its molecular weight, MW, and (optionally) its VISCOSITY; CONDUCTIVITY; and SPECIFIC_HEAT, SPECIFIC_ENTHALPY, and REFERENCE_TEMPERATURE. If either SPECIFIC_HEAT or ENTHALPY is specified, then both must be specified. The REFERENCE_TEMPERATURE is the temperature that corresponds to the specified value of SPECIFIC_ENTHALPY. In the absence of any of these parameters, the appropriate values of 'AIR' are assumed.

Recognized species that are emissive will been defined as ABSORBING and radiative absorption for those species will be computed. The keyword ABSORBING can be specified on the SPEC line as well. If .TRUE. and the species is not in the recognized list, then it will be assumed to be a fuel when invoking RADCAL to compute its absorptivity.

Table 11.1: **Optional Gas Species [8]**

Species	Mol. Wgt. (g/mol)	σ (Å)	k/ε (K)
AIR	29	3.711	78.6
ARGON	40	3.42	124.0
CARBON DIOXIDE	44	3.941	195.2
CARBON MONOXIDE	28	3.690	91.7
HELIUM	4	2.551	10.22
HYDROGEN	2	2.827	59.7
METHANE	16	3.758	148.6
NITROGEN	28	3.798	71.4
OXYGEN	32	3.467	106.7
PROPANE	44	5.118	237.1
WATER VAPOR	18	2.641	809.1

11.2.3   Special Topic: Yields of Gaseous Species (NU_GAS)

The yields of fuel and water gases are usually specified with the parameters `NU_FUEL` and `NU_WATER` on the `MATL` line. However, the yield of any explicitly-defined (via the `SPEC` line) gas species can be specified using the parameter `NU_GAS(j,k)`, where `j` refers to the `j`'th reaction of the material and `k` refers to the `k`'th explicitly-defined gas species. `NU_GAS` can also be used to specify the yields of the mixture fraction and water vapor, assuming each is implicitly-defined and its order in the list of species is obtained from the output file **CHID.out**.

For consistency, the `HEAT_OF_COMBUSTION(j,k)` can also be specified separately for each reaction and species. These values are used only if the corresponding heat of combustion for the gaseous species is greater than zero.

In the example below, the pyrolysis of wood is included within a simulation that uses a finite-rate reaction instead of the default mixture fraction model. Notice in this case that all of the gas species (except for the background nitrogen) are explicitly defined, and as a result, FDS needs to be told explicitly what gaseous species are produced by the solid phase reactions. In this case, 82 % of the mass of wood is converted to gaseous `'PYROLYZATE'` and 18 % is converted to solid `'CHAR'`.

```
&SPEC ID = 'PYROLYZATE', MW=53.6 /
&SPEC ID = 'OXYGEN', MASS_FRACTION_0 = 0.23 /
&SPEC ID = 'WATER VAPOR' /
&SPEC ID = 'CARBON DIOXIDE' /

&MATL ID = 'WOOD'
      EMISSIVITY              = 0.9
      CONDUCTIVITY            = 0.2
      SPECIFIC_HEAT           = 1.3
      DENSITY                 = 570.
      N_REACTIONS             = 1
      A                       = 1.89E10
      E                       = 1.51E5
      N_S                     = 1.0
      NU_RESIDUE              = 0.18
      NU_GAS(1,1:4)           = 0.82,0,0,0
```

```
HEAT_OF_REACTION        = 430.
HEAT_OF_COMBUSTION(1,1) = 14500.
RESIDUE                 = 'CHAR' /
```

11.2.4 Special Topic: Finite-Rate Combustion

Usually, FDS uses mixture fraction concepts to describe combustion. However, FDS can also explicitly track gas species and reactions that can occur between them. This section describes how to do this.

1. It is strongly recommended that finite-rate reactions be invoked only when FDS is running in DNS mode. Set `DNS=.TRUE.` on the `MISC` line. Note: you may use the finite-rate reaction scheme in an LES calculation, but because the temperature in a large scale calculation is smeared out over a mesh cell, some of the reaction parameters may need to be modified to account for the lower temperatures.

2. The `BACKGROUND_SPECIES` on the `MISC` line is normally set to be `'NITROGEN'`.

3. The namelist group `SPEC` is used to specify each additional species. Do not enter a `SPEC` line for the background species.

4. Read Section 11.2 for a description of the boundary conditions for the gas species.

5. The `REAC` namelist group is used to designate the fuel and the reaction rate parameters. For a finite-rate reaction you can specify multiple `REAC` lines. Note that FDS will evaluate the reactions in the order they are listed in the input file.

   `FUEL` Character string indicating which of the listed optional gas species is the fuel.

   `OXIDIZER` Character string indicating which of the listed optional gas species is the oxidizer.

   `BOF` Pre-exponential factor in one-step chemical reaction in units of cm^3/mole/s.

   `E` Activation energy for one-step chemical reaction in units of kJ/kmol.

   `NU` Array containing the stoichiometry of the chemical reaction for each `SPEC` where negative values indicate reactants and positive values indicate products. Note that the background species cannot participate in the reaction. This means that `NU(0)` is not a valid input parameter.

   `N_S` Array containing the exponents for the finite rate equation for each `SPEC`. Note that it is possible that a given `SPEC` can be assigned a value of `N_S` greater than zero and a value of `NU` equal to zero. In other words, the rate equation can be dependent on a species that does not participate directly in the reaction. Note also that the background species cannot participate in the reaction. This means that `N_S(0)` is not a valid input parameter.

   `HEAT_OF_COMBUSTION` The effective heat of combustion the chemical reaction in units of kJ/kg. (Default 40,000 kJ/kg)

11.3 Radiation Transport: The `RADI` Namelist Group

For most FDS simulations, thermal radiation transport is computed by default and you need not set any parameters to make this happen. However, there are situations where it is important to be aware of issues related to the radiative transport solver. The most important issue involves the fraction of energy released from the fire as thermal radiation, commonly referred to as the *radiative fraction*. It is a function of both the flame temperature and chemical composition, neither of which are reliably calculated in a large scale fire calculation because the flame sheet is not well-resolved. In calculations in which the mesh cells are on the order of a centimeter or larger, the temperature near the flame surface cannot be relied upon when computing the source term in the radiation transport equation, especially because of the T^4 dependence. As a practical alternative, the parameter `RADIATIVE_FRACTION` on the `RADI` line allows you to specify explicitly the fraction of the total combustion energy that is released in the form of thermal radiation. Some of that energy may be reabsorbed elsewhere, yielding a net radiative loss from the fire or compartment that is less than the `RADIATIVE_FRACTION`, depending mainly on the size of the fire and the soot loading. If it is desired to use the radiation transport equation as is, then `RADIATIVE_FRACTION` ought to be set to zero, and the source term in the radiative transport equation is then based solely on the gas temperature and the chemical composition. By default, the `RADIATIVE_FRACTION` is 0.35 for an LES calculation, and zero for DNS.

There are several ways to improve the performance of the Finite Volume Method in solving the radiation transport equation (RTE), most of which increase the computation time. The solver has two modes of operation – a gray gas model (default) and a wide band model [5]. Modifications to these models can be made via parameters on the `RADI` line. If running in gray gas mode (default), increase the number of angles from the default 100 with the integer parameter `NUMBER_RADIATION_ANGLES`. The frequency of calls to the radiation solver can be reduced from every 3 time steps with integer called `TIME_STEP_INCREMENT`. The increment over which the angles are updated can be reduced from 5 with the integer called `ANGLE_INCREMENT`. Briefly, if `TIME_STEP_INCREMENT` and `ANGLE_INCREMENT` are both set to 1, the radiation field is completely updated in a single time step, but the cost of the calculation increases significantly.

A few parameters affecting the absorption of radiation by water droplets are as follows: `RADTMP` is the assumed radiative source temperature. It is used in the computation of the mean scattering and absorption cross sections of water droplets. The default is 900 °C. `NMIEANG` is the number of angles in the numerical integration of the Mie-phase function. Increasing `NMIEANG` improves the accuracy of the radiative properties of water droplets. The cost of the better accuracy is seen in the initialization phase, not during the actual simulation. The default value for `NMIEANG` is 15.

If the optional six band model is desired, set `WIDE_BAND_MODEL=.TRUE.`. It is recommended that this option only be used when the fuel is relatively non-sooting because it adds significantly to the cost of the calculation. To add three additional fuel bands, set `CH4_BANDS=.TRUE.`. See FDS Technical Reference Guide for more details. Note also that when `WIDE_BAND_MODEL=.TRUE.`, the `ABSORPTION_COEFFICIENT` output quantity becomes practically useless, because it then corresponds to one individual band of the spectrum.

It is possible to turn off the radiation transport solver (saving roughly 20 % in CPU time) by adding the statement `RADIATION=.FALSE.` to the `MISC` line. For isothermal calculations, the radiation is turned off automatically. If burning is taking place and radiation is turned off, then the total heat release rate is reduced by the `RADIATIVE_FRACTION`, which is input on the `RADI` line. This radiated energy completely disappears from the calculation. More on this feature can be found in Section 11.1.2.

In simulations with no combustion nor radiating species, it is possible to use a constant absorption coefficient by specifying `KAPPA0` on the `RADI` line.

Chapter 12

Particles and Droplets

Lagrangian particles[1] are used in FDS to represent water or liquid fuel droplets, flow tracers, and various other objects that are not defined or confined by the numerical mesh. Sometimes the particles have mass, sometimes they do not. Some evaporate, absorb radiation, *etc.* PART is the namelist group that is used to prescribe parameters associated with Lagrangian particles.

All Lagrangian particles must be explicitly defined via the PART namelist group. In versions of FDS prior to 5, water droplets and smoke particles were implicitly defined. Shortcuts for defining water droplets and smoke particles are possible, via parameters like WATER=.TRUE. and MASSLESS=.TRUE.

12.1 Basics

Properties of different types of Lagrangian particles are designated via the PART namelist group. Once a particular type of particle or droplet has been described using a PART line, then the name of that particle or droplet type is invoked elsewhere in the input file via the parameter PART_ID. There are no reserved PART_IDs – all must be defined. For example, an input file may have several PART lines that include the properties of different types of Lagrangian particles:

```
&PART ID='my smoke',... /
&PART ID='my water',... /
```

These Lagrangian particles can be introduced at a solid surface via the SURF line that defines the properties of the material, for example

```
&SURF ...,PART_ID='my smoke' /
```

or the PART_ID can be invoked from a PROP line to change the properties of the droplets ejected by a sprinkler or nozzle, for example

```
&PROP ID='Acme Spk-123', QUANTITY='SPRINKLER LINK TEMPERATURE', PART_ID='my water', ... /
```

---

[1]Throughout this section, the terms "droplets" and "particles" are used interchangeably. From the point of view of FDS, they are all Lagrangian particles; that is, point elements that are not bound by the structure of the underlying grid.

12.2 Particle and Droplet Insertion

12.2.1 Controlling the Number of Particles and Droplets

Regardless of how the particles or droplets are introduced into the computational domain, the following are important parameters for controlling their number:

DT_INSERT Time increment in seconds between the introduction of a "batch" of particles or droplets. The number per "batch" depends on how they are introduced. If more particles are desired, lower the input value of this parameter. The default value is 0.01 s.

SAMPLING_FACTOR Sampling factor for the output file **CHID.prt5**. This parameter can be used to reduce the size of the particle output file used to animate the simulation. The default value is 1 for MASSLESS particles, meaning that every particle or droplet will be shown in Smokeview. The default is 10 for all other types of particles. MASSLESS particles are discussed in Section 12.4.

AGE Number of seconds the particle or droplet exists, after which time it is removed from the calculation. This is a useful parameter to use when trying to reduce the number of droplets or particles in a simulation.

12.2.2 Particles Introduced at a Solid Surface

If the particles have mass and are introduced from a solid surface, specify PARTICLE_MASS_FLUX on the SURF line. The number of particles inserted at each solid cell every DT_INSERT seconds is specified by NPPC on the SURF line defining the solid surface. The default value of NPPC is 1. As an example, the following set of input lines:

```
&PART ID='drops', QUANTITIES(1:3)='DROPLET_DIAMETER','DROPLET_TEMPERATURE','DROPLET_AGE',
      DIAMETER=750., SAMPLING_FACTOR=1, COLOR='RED', EVAPORATE=.FALSE. /
&SURF ID='HOLE', PART_ID='drops', VEL=-5., PARTICLE_MASS_FLUX=0.1, COLOR='RED' /
&OBST XB=-0.2,0.2,-0.2,0.2,4.0,4.4, SURF_IDS='INERT','HOLE','INERT' /
```

creates an obstruction that ejects non-evaporating, red particles with a mean volumetric diameter of 750 μm out of its sides at a rate of 0.1 kg/m^2/s. FDS will adjust the mass flux if the obstruction or vent dimensions are changed to conform to the numerical grid. Note that the IDs have no meaning other than as identifiers. The particles are colored red in Smokeview, but can also be colored according to their diameter, temperature, or age.

Note that a surface on which particles are specified must have a non-zero normal velocity directed into the computational domain. This happens automatically if the surface is burning, but must be specified if it is not.

12.2.3 Droplets Introduced at a Sprinkler or Nozzle

DROPLETS_PER_SECOND is the number of droplets inserted every second per active sprinkler or nozzle (Default 5000). Note that this parameter only affects sprinklers and nozzles. Changing this parameter does *not* change the flow rate, but rather the number of droplets used to represent the flow. Also note that the number of droplets introduced per "batch" is DROPLETS_PER_SECOND times DT_INSERT.

Note that `DROPLETS_PER_SECOND` can be a very important parameter. In some simulations, it is a good idea to increase this number so that the liquid mass is distributed more uniformly over the droplets. If this parameter is too small, it can lead to a non-physical evaporation pattern, sometimes even to the point of causing a numerical instability. If you encounter a numerical instability shortly after the activation of a sprinkler or nozzle, consider increasing `DROPLETS_PER_SECOND` to produce a smoother evaporation pattern that is more realistic. Keep in mind that for a real sprinkler or nozzle, there are many more droplets created per second than the number that can be simulated.

12.2.4 Particles or Droplets Introduced at the Start of the Calculation

Sometimes it is convenient to introduce droplets or particles at the start of the simulation. For this purpose, `NUMBER_INITIAL_DROPLETS` is the number of particles/droplets within the computational domain at the start of the simulation. Its default value is 0, meaning that initially there are no particles or droplets present. If non-zero, also specify `MASS_PER_VOLUME` (kg/m^3) which specifies the particle/droplet mass per unit volume (Default 1 kg/m^3). Do not confuse this parameter with `DENSITY`, explained in the next section. For example, water has a `DENSITY` of 1000 kg/m^3, whereas a liter of water broken up into droplets and spread over a cubic meter has a `MASS_PER_VOLUME` of 1 kg/m^3. Also, to limit the particles/droplets to a certain region of the domain, add the real sextuplet `XB` to designate the coordinates of a rectangular volume. The format for `XB` is the same as that used on the `OBST` line.

12.2.5 Droplets that Strike Solid Surfaces

When a droplet strikes a solid surface, it sticks and is reassigned a new speed and direction. If the surface is horizontal, the direction is randomly chosen. If vertical, the direction is downwards. The rate at which the droplets move over the horizontal and vertical surfaces is difficult to quantify. The parameters `HORIZONTAL_VELOCITY` and `VERTICAL_VELOCITY` on the `PART` line allow you to control the rate at which droplets move horizontally or vertically (downward). The defaults are 0.2 m/s and 0.5 m/s, respectively.

There are some applications, like the suppression of racked storage commodities, where it is useful to allow water droplets to move horizontally along the underside of a solid object. It is difficult to model this phenomenon precisely because it involves surface tension, surface porosity and absorption, and complicated geometry. However, a way to capture some of the effect is to set `ALLOW_UNDERSIDE_DROPLETS=.TRUE.` on the `MISC` line. It is normally false.

Be aware that when droplets hit obstructions, the vertical direction is assumed to coincide with the z axis, regardless of any change to the gravity vector, `GVEC`.

A useful sample case to demonstrate various features of droplet motion on solid obstructions is the test case called **cascade.fds**. Figure 12.1 shows a stream of water droplets impinging on the top of a box followed by the cascading of water droplets over the top edge.

12.3 Particle and Droplet Properties

12.3.1 Thermal Properties

For Lagrangian particles that are not `MASSLESS`, the following parameters should be included on the `PART` line to indicate how they heat up and possibly evaporate. It is assumed by default that non-massless particles are liquid droplets, but you can specify `EVAPORATE=.FALSE.` to change this.
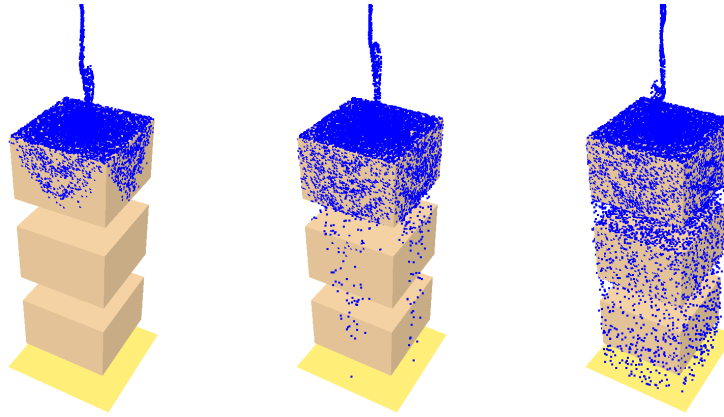
Figure 12.1: Smokeview rendering of the **cascade** test case.

DENSITY The density of the liquid or solid droplet/particle. (Default 1000 kg/m^3)

SPECIFIC_HEAT Specific heat of liquid or solid droplet/particle. (Default 4.184 kJ/kg/K)

VAPORIZATION_TEMPERATURE Boiling temperature of liquid droplet. (Default 100 °C)

MELTING_TEMPERATURE Melting (solidification) temperature of liquid droplet. (Default 0 °C)

INITIAL_TEMPERATURE Initial temperature of liquid droplet. (Default TMPA)

HEAT_OF_VAPORIZATION Latent heat of vaporization of liquid droplet. (Default 2259 kJ/kg)

Notice that the default thermal properties are that of water, and also notice that there is no specified thermal conductivity because the droplets are assumed to be thermally-thin.

12.3.2 Size Distribution

The DIAMETER is the median volumetric diameter of the droplets or particles, with the distribution assumed to be a combination of Rosin-Rammler and log-normal (Default 500 μm). The width of the distribution is controlled by the parameter GAMMA_D (default 2.4) The Rosin-Rammler/log-normal distribution is given by

$$F(d) = \begin{cases} \frac{1}{\sqrt{2\pi}} \int_0^d \frac{1}{\sigma d'} e^{-\frac{[\ln(d'/d_m)]^2}{2\sigma^2}} \, dd' & (d \leq d_m) \\ 1 - e^{-0.693\left(\frac{d}{d_m}\right)^\gamma} & (d_m < d) \end{cases} \tag{12.1}$$

Note that the parameter σ is given the value $\sigma = 2/(\sqrt{2\pi}(\ln 2)\gamma) = 1.15/\gamma$ which ensures that the two functions are smoothly joined at $d = d_m$. You can also add a value for SIGMA_D to the PART line if you want to over-ride this feature. The larger the value of γ, the narrower the droplet size is distributed about the median value. Note that you can prevent droplets or particles from exceeding MAXIMUM_DIAMETER, which is infinitely large by default. Also note that droplets less than MINIMUM_DIAMETER are assumed to evaporate in a single time step, eliminating numerical instabilities that can occur when droplets get very, very small. The default MINIMUM_DIAMETER is 20 μm. To prevent FDS from generating a distribution of droplets/particles altogether, set MONODISPERSE=.TRUE. on the PART line, in which case every droplet or particle will be assigned the same DIAMETER.

12.3.3 Color

The parameter `QUANTITIES` is an array of character strings indicating which scalar quantities should be used to color the particles or droplets when viewed as an animation. The choices are

`'DROPLET_TEMPERATURE'` ($^\circ$C)
`'DROPLET_DIAMETER'` (μm)
`'DROPLET_VELOCITY'` (m/s)
`'DROPLET_MASS'` (kg)
`'DROPLET_AGE'` (s)

As a default, if no `QUANTITIES` are specified and none are selected in Smokeview, then Smokeview will display particles with a single color. To select this color specify either `RGB` or `COLOR`. By default, water droplets are colored blue and fuel droplets yellow. All others are colored black.

12.4 Special Types of Particles and Droplets

There are several useful attributes that you can assign to particles or droplets, usually via a simple logical parameter. Be aware with each of these parameters that specifying it as `.TRUE.` may cause other parameters to be functionally useless, or may cause conflicts that FDS may or may not detect. A good rule of thumb is always to ask yourself what is the basic information that *must* be conveyed to the program, and stick to that. For example, if the particles are to be `MASSLESS`, there is no point in declaring thermal properties because they are only to be used a flow tracers in Smokeview.

12.4.1 Massless Particles

The simplest use of Lagrangian particles is for visualization, in which case the particles are considered massless tracers. In this case, the particles are defined via the line

```
&PART ID='tracers', MASSLESS=.TRUE., ... /
```

Note that if the particles are `MASSLESS`, it is not appropriate to color them according to any particular property. Unlike early versions of FDS, particles are no longer colored by gas phase quantities, but rather by properties of the particle itself. For example, `'DROPLET_TEMPERATURE'` for a non-massless particle refers to the temperature of the particle itself rather than the local gas temperature.

Also note that if `MASSLESS=.TRUE.`, the `SAMPLING_FACTOR` is set to 1 unless you say otherwise, which would be pointless since `MASSLESS` particles are for visualization only.

12.4.2 Static Particles or Droplets

`STATIC` is a logical parameter indicating whether particles move or just serve as obstructions or clutter. Setting `STATIC=.TRUE.` only makes sense in conjunction with a non-zero value of `NUMBER_INITIAL_DROPLETS`. The default value of `STATIC` is `.FALSE.`

12.4.3 Water Droplets

`WATER=.TRUE.` declares that the liquid droplets evaporate into `'WATER VAPOR'`, a separate gas species that is *automatically* added to the calculation by this command. By default, `WATER=.FALSE.`, even though the default properties of droplets are that of water. Setting `WATER=.TRUE.` instructs FDS to add `'WATER VAPOR'` as an explicitly defined species, and it also invokes appropriate constants related to the absorption of thermal radiation by the water droplets. It also causes the droplets to be colored blue in Smokeview.

If the liquid droplets are to evaporate into some other gaseous species, you must explicitly define the species via the SPEC namelist group (see Section 11.2), and then designate the appropriate SPEC_ID on the PART line.

12.4.4 Fuel Droplets

FUEL=.TRUE. indicates that the liquid droplets evaporate into fuel gas and burn. In this case, add the HEAT_OF_COMBUSTION (kJ/kg) of the fuel to the PART line. Fuel droplets are colored yellow by default in Smokeview. This feature only works for a mixture fraction-based combustion calculation, in which case the droplets evaporate into an equivalent amount of fuel vapor such that the resulting heat release rate (assuming complete combustion) is equal to the evaporation rate multiplied by the HEAT_OF_COMBUSTION. If a spray nozzle is used to generate the fuel droplets, its characteristics are specified in the same way as those for a sprinkler.

Example Case: spray_burner

Controlled fire experiments are often conducted using a spray burner, where a liquid fuel is sprayed out of a nozzle and ignited. In this example (**spray_burner.fds**), heptane from two nozzles is sprayed downwards into a steel pan. The flow rate is increased linearly so that the fire grows to 2 MW in 20 s, burns steadily for another 20 s, and then ramps down linearly in 20 s. The key input parameters are given here:

```
&DEVC ID='nozzle_1', XYZ=4.0,-.3,0.5, PROP_ID='nozzle', QUANTITY='TIME', SETPOINT=0. /
&DEVC ID='nozzle_2', XYZ=4.0,0.3,0.5, PROP_ID='nozzle', QUANTITY='TIME', SETPOINT=0. /

&PART ID='heptane droplets', FUEL=.TRUE., VAPORIZATION_TEMPERATURE=98.,
      HEAT_OF_VAPORIZATION=316., SPECIFIC_HEAT=2.25, DENSITY=688.,
      QUANTITIES(1:2)='DIAMETER','DROPLET_TEMPERATURE',
      DROPLETS_PER_SECOND=2000, DIAMETER=1000., HEAT_OF_COMBUSTION=44500.,
      DT_INSERT=0.02, SAMPLING_FACTOR=1 /

&PROP ID='nozzle', CLASS='NOZZLE', PART_ID='heptane droplets',
      FLOW_RATE=1.96, FLOW_RAMP='fuel', DROPLET_VELOCITY=10.,
      SPRAY_ANGLE=0.,30.    /
&RAMP ID='fuel', T= 0.0, F=0.0  /
&RAMP ID='fuel', T=20.0, F=1.0  /
&RAMP ID='fuel', T=40.0, F=1.0  /
&RAMP ID='fuel', T=60.0, F=0.0  /
```

Many of these parameters are self-explanatory. Note that a 2 MW fire is achieved via 2 nozzles flowing heptane at 1.96 L/min each:

$$2 \times 1.96 \; \frac{\text{L}}{\text{min}} \times \frac{1}{60} \; \frac{\text{min}}{\text{s}} \times 688 \; \frac{\text{kg}}{\text{m}^3} \times \frac{1}{1000} \; \frac{\text{m}^3}{\text{L}} \times 44500 \; \frac{\text{kJ}}{\text{kg}} = 2000 \, \text{kW} \quad (12.2)$$

The parameter HEAT_OF_COMBUSTION over-rides that for the overall reaction scheme. Thus, if other droplets or solid objects have different heats of combustion, the effective burning rates are adjusted so that the total heat release rate is that which the user expects. However, exercises like this ought to be conducted just to ensure that this is the case. The HRR curve for this example is given in Fig. 12.2.

Note that FUEL=.TRUE. automatically invokes a mixture fraction calculation in which fuel from the evaporating fuel droplets is burned according to the overall reaction scheme. Because the default mixture fraction combustion model assumes that fuel and oxygen burn when mixed (assuming that the oxygen concentration is above an empirically determined threshold), there is no need to specify an ignition source. For
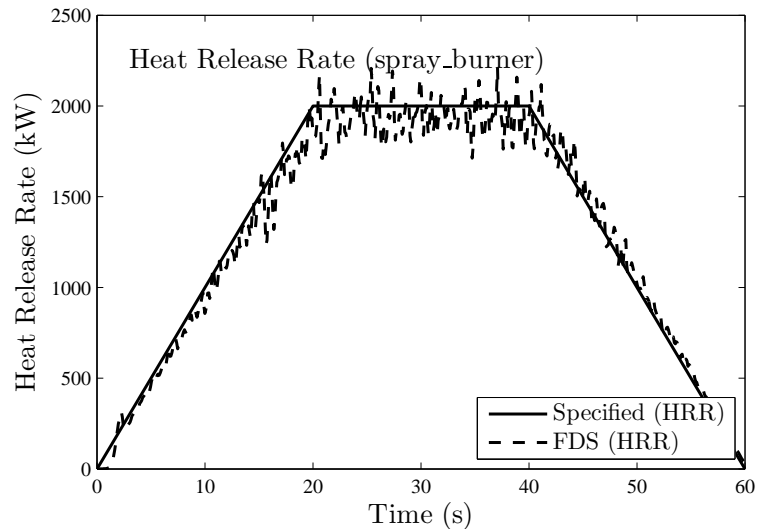
Figure 12.2: Heat Release Rate (HRR) of spray burner test.

most liquid fuels, the small amount of evaporation at ambient temperature is enough to start the combustion process. In some sense, there is an implicit pilot flame.

Note also that this feature is subject to mesh dependence. If the mesh cells are too coarse, the evaporating fuel can be diluted to such a degree that it may not burn. Proper resolution depends on the type of fuel and the amount of fuel being ejected from the nozzle. Always test your burner at the resolution of your overall simulation.

12.4.5 Solid Particles that do not Evaporate

Unless you declare `MASSLESS=.TRUE.` on the `PART` line, it is assumed that the particle or droplet has mass and thermal properties that govern its heating and evaporation. To prevent evaporation, set `EVAPORATE=.FALSE.`. The particles will still heat up due to convection, but they will not shrink and no additional gaseous species need to be declared.

Note that the absorption of thermal radiation by water (`WATER=.TRUE.`) or fuel droplets (`FUEL=.TRUE.`) is handled in FDS with fairly well-established physical sub-models, the details of which are contained in the FDS Technical Reference Guide [5]. However, for arbitrary particles or droplets, there is no assumed radiative absorption.

12.5 Special Topic: Suppression by Water (Mixture Fraction Model Only)

Modeling suppression of a fire by a water spray is challenging because the relevant physical mechanisms occur at length scales smaller than a single mesh cell. In the gas phase, flames are extinguished due to lowered temperatures and dilution of the oxygen supply. See Section 11.1.2 for more information about gas phase suppression.

For the solid phase, water reduces the fuel pyrolysis rate by cooling the fuel surface and also changing the chemical reactions that liberate fuel gases from the solid. If the solid or liquid fuel has been given reaction parameters via the MATL line, there is no need to set any additional suppression parameters. It is assumed that water impinging on the fuel surface takes energy away from the pyrolysis process and thereby reduces the burning rate of the fuel. If the surface has been assigned a HRRPUA (Heat Release Rate Per Unit Area), a parameter needs to be specified that governs the suppression of the fire by water because this type of simulated fire essentially acts like a gas burner whose flow rate is explicitly specified. An empirical way to account for fire suppression by water is to characterize the reduction of the pyrolysis rate in terms of an exponential function. The local mass loss rate of the fuel is expressed in the form

$$\dot{m}''_f(t) = \dot{m}''_{f,0}(t)\, e^{-\int k(t)\, dt} \tag{12.3}$$

Here $\dot{m}''_{f,0}(t)$ is the user-specified burning rate per unit area when no water is applied and k is a function of the local water mass per unit area, m''_w, expressed in units of kg/m^2.

$$k(t) = \texttt{E\_COEFFICIENT}\, m''_w(t) \quad \text{s}^{-1} \tag{12.4}$$

The parameter E_COEFFICIENT must be obtained experimentally, and it is expressed in units of m^2/kg/s. Usually, this type of suppression algorithm is invoked when the fuel is complicated, like a cartoned commodity.

Chapter 13

Devices and Control Logic

Sprinklers, smoke detectors, heat flux gauges, and thermocouples may seem to be completely unrelated, but from the point of view of FDS, they are simply devices that operate in specific ways depending on the properties assigned to them. They can be used to record some quantity of the simulated environment, like a thermocouple, or they can represent a mathematical model of a complex sensor, like a smoke detector, and in some cases they can trigger events to happen, like a timer.

Versions of FDS prior to FDS 5 used device-specific namelist groups, like `SPRK`, `HEAT`, `SMOD`, and `THCP`, but the number and variety of fire-specific sensing and measurement devices continues to expand, and the data structures in FDS could not easily accommodate all possibilities. In addition, the logic associated with sensor activation and subsequent actions, like a vent opening, had become too complicated and prone to bugs. Starting in FDS 5, all devices, in the broadest sense of the word, are designated via the namelist group `DEVC`. In addition, advanced functionality and properties are accommodated via additional namelists groups called `CTRL` (Control) and `PROP` (Properties).

13.1 Device Location and Orientation: The `DEVC` Namelist Group (Table 15.4)

Regardless of the specific properties, each device needs to be sited either at a point within the computational domain, or over a span of the domain, like a beam smoke detector. For example, a sprinkler is sited within the domain with a line like:

```
&DEVC XYZ=3.0,5.6,2.3, PROP_ID='Acme Sprinkler 123', ID='Spk_39' /
```

The physical coordinates of the device are given by a triplet of real numbers, `XYZ`. The properties of the device are contained on the `PROP` line designated by `PROP_ID`, which will be explained below for each of the special devices included in FDS. The character string `ID` is merely a descriptor to identify the device in the output files, and if any action is tied to its activation.

Not all devices need to be associated with a particular set of properties via the `PROP_ID`. For example, pointwise output quantities are specified with a single `DEVC` line, like

```
&DEVC ID='TC-23', XYZ=3.0,5.6,2.3, QUANTITY='TEMPERATURE'  /
```

which tells FDS to record the temperature at the given point as a function of time. The `ID` is a label in the output file whose name is **CHID_devc.csv**.

Some devices have a particular orientation which can be specified with various parameters; `IOR`, `ORIENTATION`, `ROTATION`. `IOR` or the Index of Orientation, is necessary for any device that is placed on the surface of a

solid. The values ±1 or ±2 or ±3 indicate the direction that the device "points", where 1 is parallel to the *x*-axis, 2 is parallel to the *y*-axis and 3 is parallel to the *z*-axis.

ORIENTATION is used for devices that are not on a surface and require a directional specification, like a sprinkler. ORIENTATION is specified with a triplet of real number values that indicate the components of the direction vector. The default value of ORIENTATION is (0,0,-1). For example, a default downward-directed sprinkler spray can be redirected in other direction. If you were to specify

```
&DEVC XYZ=3.0,5.6,2.3, PROP_ID='...', ID='...', ORIENTATION=1,0,0 /
```

the sprinkler would point in the positive *x* direction. For other devices, the ORIENTATION would only change the way the device is drawn by Smokeview.

13.2 Device Output

Each device has a QUANTITY associated with it. The output file for all DEVC quantities is a comma-delimited ASCII file called **CHID_devc.csv** (See Section 19.3 for output file format). This file can be imported into most spread sheet software packages. If the number of DEVC lines exceeds 256, the limit of some spreadsheet applications, the output file will be split into appropriately sized smaller files. To prevent the file splitting, specify COLUMN_DUMP_LIMIT=.FALSE. on the DUMP line.

By default, the DEVC output is written to a file every DT_DEVC seconds. This time increment is specified on the DUMP line. Also, by default, a time-averaged value is written out for each quantity of interest. To prevent FDS from time-averaging the DEVC output, add TIME_AVERAGED=.FALSE. to the DEVC line.

All devices must have a specified QUANTITY. Some special devices (Section 13.3) have their QUANTITY specified on a PROP line. A QUANTITY specified on a PROP line associated with a DEVC line will override a QUANTITY specified on the DEVC line.

13.3 Special Devices and their Properties: The `PROP` Namelist Group (Table 15.17)

Many devices are fairly easy to describe, like a point measurement, with only a few parameters which can be included on the `DEVC` line. However, for more complicated devices, it is inconvenient to list all of the properties on each and every `DEVC` line. For example, a simulation might include hundreds of sprinklers, but it is tedious to list the properties of the sprinkler each time the sprinkler is sited. For these devices, use a separate namelist group called `PROP` to store the relevant parameters. Each `PROP` line is identified by a unique `ID`, and invoked by a `DEVC` line by the string `PROP_ID`. The `ID` might be the manufacturer's name, like `'ACME Sprinkler 123'`, for example.

The best way to describe the `PROP` group is to list the various special devices and their properties.

13.3.1 Sprinklers

Here is a very simple example of sprinkler:

```
&PROP ID='K-11', QUANTITY='SPRINKLER LINK TEMPERATURE', RTI=148., C_FACTOR=0.7,
      ACTIVATION_TEMPERATURE=74., OFFSET=0.10,PART_ID='water drops', FLOW_RATE=189.3,
      DROPLET_VELOCITY=10., SPRAY_ANGLE=30.,80.   /

&DEVC ID='Spr_60', XYZ=22.88,19.76,7.46, PROP_ID='K-11' /
&DEVC ID='Spr_61', XYZ=22.88,21.76,7.46, PROP_ID='K-11' /
```

A sprinkler, known as `'Spr_60'`, is located at a point in space given by `XYZ`. It is a `'K-11'` type sprinkler, whose properties are given on the `PROP` line. Note that the various names (`ID`s) mean nothing to FDS, except as a means of associating one thing with another, so try to use `ID`s that are as meaningful to you as possible. The parameter `QUANTITY='SPRINKLER LINK TEMPERATURE'` *does* have a specific meaning to FDS, directing it to compute the activation of the device using the standard RTI algorithm. The various sprinkler properties will be discussed below. [1]

Properties associated with sprinklers included in the `PROP` group are:

`RTI` Response Time Index in units of $\sqrt{\text{m} \cdot \text{s}}$. (Default 100.)

`C_FACTOR` in units of $\sqrt{\text{m/s}}$. (Default 0.)

`ACTIVATION_TEMPERATURE` in units of °C. (Default 74 °C)

`INITIAL_TEMPERATURE` of the link in units of °C. (Default `TMPA`)

`FLOW_RATE` in units of L/min. An alternative is to provide the `K_FACTOR` in units of L/min/bar$^{\frac{1}{2}}$ and the `OPERATING_PRESSURE` in units of atm. The flow rate is then given by $\dot{m}_w = K\sqrt{p}$. Note that 1 bar is equivalent to 14.5 psi, 1 gpm is equivalent to 3.785 L/min, 1 gpm/psi$^{\frac{1}{2}}$ is equivalent to 14.41 L/min/bar$^{\frac{1}{2}}$.

`OFFSET` Radius of a sphere (m) surrounding the sprinkler where the water droplets are initially placed in the simulation. It is assumed that at and beyond the `OFFSET` the droplets have completely broken up and are transported independently of each other. (Default 0.05 m)

`DROPLET_VELOCITY` Initial droplet velocity. (Default 0 m/s)

---

[1]Prior to FDS 5, a separate file was used to store properties of a given sprinkler. This file is no longer used.

ORIFICE_DIAMETER Diameter of the nozzle orifice in m (default 0 m). This input provides an alternative way to set droplet velocity by giving values for FLOW_RATE and ORIFICE_DIAMETER, in which case the the droplet velocity is computed by dividing the flow rate by the orifice area. Use this method if you do not have any information about droplet velocity. However, quite often the user must fine-tune DROPLET_VELOCITY in order to reproduce certain spray profile. The ORIFICE_DIAMETER input is not used if either DROPLET_VELOCITY or SPRAY_PATTERN_TABLE is specified.

SPRAY_ANGLE A pair of angles (in degrees) through which the droplets are sprayed. The angles outline a conical spray pattern relative to the south pole of the sphere centered at the sprinkler with radius OFFSET. For example, SPRAY_ANGLE=30.,80. directs the water droplets to leave the sprinkler through a band between $60°$ and $10°$ south latitude, assuming the orientation of the sprinkler is (0,0,-1), the default. The droplets are uniformly distributed within this belt.

SPRAY_PATTERN_TABLE Name of a set of TABL lines containing the description of the spray pattern.

PART_ID The name of the PART line containing properties of the droplets. See Chapter 12 for additional details.

PRESSURE_RAMP The name of the RAMP lines specifying the dependence of pipe pressure on the number of active sprinklers and nozzles.

Be aware that sprinklers produce many droplets that need to be tracked in the calculation. To limit the computational cost, sprinkler droplets disappear when they hit the lower boundary of the computational domain, regardless of whether it is solid or not. To stop FDS from removing sprinkler droplets from the lower boundary of the computational domain, add the phrase POROUS_FLOOR=.FALSE. to the MISC (Section 6.4) line. Be aware, however, that droplets that land on the floor continue to move horizontally in randomly selected directions; bouncing off obstructions, and consuming CPU time.

   For more information about sprinklers, their activation and spray dynamics, read the FDS Technical Reference Guide [5].

Special Topic: Specifying Complex Spray Patterns

If a more complex spray pattern is desired than can be achieved by using SPRAY_ANGLE, DROPLET_VELOCITY, and FLOW_RATE, then a SPRAY_PATTERN_TABLE can be specified using the TABL (Section 10) namelist group. For a spray pattern, specify the total flow using FLOW_RATE of the PROP line, the name of the spray pattern using SPRAY_PARTTERN_TABLE and then one or more TABL lines of the format:

```
&TABL ID='table_id', TABLE_DATA=LAT1,LAT2,LON1,LON2,VELO,FRAC /
```

where each TABL line for a given 'table_id' provides information about the spherical distribution of the spray pattern for a specified solid angle. LAT1 and LAT2 are the bounds of the solid angle measured in degrees from the south pole (0 is the south pole and 90 is the equator, 180 is the north pole). Note that this is not the conventional way of specifying a latitude, but rather a convenient system based on the fact that a typical sprinkler sprays water downwards, which is why 0 degrees is assigned to the "south pole," or the $-z$ direction. The parameters LON1 and LON2 are the bounds of the solid angle (also in degrees), where 0 (or 360) is aligned with the $-x$ axis and 90 is aligned with the $-y$ axis. VELO is the velocity (m/s) of the droplets at their point of insertion. FRAC the fraction of the total flow rate of liquid that should emerge from that particular solid angle.

   In the test case called **bucket_test_2**, the spray pattern is defined as two jets, each with a velocity of 10 m/s and a flow rate of 60 L/min. The first jet contains 0.2 of the total flow, the second, 0.8 of the total. The jets are centered at points $30°$ below the "equator," and are separated by $180°$.

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```
&PROP ID='K-11', QUANTITY='SPRINKLER LINK TEMPERATURE', OFFSET=0.10, PART_ID='water_drops',
      FLOW_RATE=60.,SPRAY_PATTERN_TABLE='TABLE1', SMOKEVIEW_ID='sprinkler_upright',
      DROPLET_VELOCITY=10. /

&TABL ID='TABLE1',TABLE_DATA=30,31,0,1,5,0.2/
&TABL ID='TABLE1',TABLE_DATA=30,31,179,180,5,0.8/
```

Note that each set of TABL lines must have a unique ID. Also note that the TABL lines can be specified in any order.

Special Topic: Varying Pipe Pressure

In real sprinkler systems, the pipe pressure is affected by the number of actuated sprinklers. Typically, the pressure is higher than the design value when the first sprinkler activates, and decreases towards the design value and below that when more and more sprinklers are activated. The pipe pressure has an effect on flow rate, droplet velocity and droplet size distribution.

In FDS, the varying pipe pressure can be specified on a PROP line using PRESSURE_RAMP. On each RAMP line, the number of open sprinklers or nozzles is associated with certain pipe pressure (atm). For example:

```
&PROP ID='My nozzle'
      OFFSET=0.1
      PART_ID='water drops'
      FLOW_RATE=0.9
      OPERATING_PRESSURE = 10.0
      DROPLET_VELOCITY=15.0
      SPRAY_ANGLE=0.0,80.0
      PRESSURE_RAMP = 'PR1' /

&RAMP ID = 'PR1' T = 1, F = 16.0 /
&RAMP ID = 'PR1' T = 2, F = 10.0 /
&RAMP ID = 'PR1' T = 3, F = 8.0 /
```

These lines would indicate that the pressure is 16.0 atm when the first sprinkler having properties of My nozzle activates, 10.0 atm when two sprinklers are active, and 8.0 atm when three or more sprinklers are active. When counting the number of active sprinklers, FDS accounts for all active sprinklers or nozzles with PART_ID associated with them.

When pressure ramps are used, both FLOW_RATE and DROPLET_VELOCITY are associated with the OPERATING_PRESSURE. Specify either the FLOW_RATE, or the K_FACTOR and OPERATING_PRESSURE. In the latter case, the flow rate is given by $\dot{m}_w = K\sqrt{p}$ and droplet velocity by $v = C\sqrt{p}$. If spray pattern table is used, the coefficient C is determined separately for each line of the table. The median diameter of the particle size distribution is scaled as $d_m(p) = d_m(p_o)(p_o/p)^{1/3}$, where p_o is the OPERATING_PRESSURE and $d_m(p_o)$ is specified by parameter DIAMETER on the corresponding PART line.

13.3.2 Nozzles

Nozzles are very much like sprinklers, only they do not activate based on the standard RTI model. To simulate a nozzle that activates at a given time, specify a QUANTITY and SETPOINT directly on the DEVC line. The following lines:

```
&DEVC XYZ=23.91,21.28,0.50, PROP_ID='nozzle', ORIENTATION=0,0,1, QUANTITY='TIME',
      SETPOINT=0., ID='noz_1' /
&DEVC XYZ=26.91,21.28,0.50, PROP_ID='nozzle', ORIENTATION=0,0,1, QUANTITY='TIME',
      SETPOINT=5., ID='noz_2' /
&PROP ID='nozzle', PART_ID='heptane drops', FLOW_RATE=2.132,
      FLOW_TAU=-50., DROPLET_VELOCITY=5., SPRAY_ANGLE=0.,45.    /
```

designate two nozzles of the same type, one which activates at time zero, the other at 5 s. Note that nozzles must have a designated PROP_ID, and the PROP line must have a designated PART_ID to describe the liquid droplets.

13.3.3   Heat Detectors

QUANTITY='LINK TEMPERATURE' defines a heat detector, which uses essentially the same activation algorithm as a sprinkler, without the water spray.

```
&DEVC ID='HD_66', PROP_ID='Acme Heat', XYZ=2.3,4.6,3.4 /
&PROP ID='Acme Heat', QUANTITY='LINK TEMPERATURE', RTI=132., ACTIVATION_TEMPERATURE=74. /
```

Like a sprinkler, RTI is the Response Time Index in units of $\sqrt{\text{m} \cdot \text{s}}$. ACTIVATION_TEMPERATURE is the link activation temperature in degrees C (Default 74 °C). INITIAL_TEMPERATURE is the initial temperature of the link in units of °C (Default TMPA).

13.3.4   Smoke Detectors

A smoke detector is defined in the input file with an entry similar to:

```
&DEVC ID='SD_29', PROP_ID='Acme Smoke Detector', XYZ=2.3,4.6,3.4 /
&PROP ID='Acme Smoke Detector', QUANTITY='CHAMBER OBSCURATION', LENGTH=1.8,
      ACTIVATION_OBSCURATION=3.28 /
```

for the single parameter Heskestad model. Note that a PROP line is mandatory for a smoke detector, in which case the DEVC QUANTITY can be specified on the PROP line. For the four parameter Cleary model, use a PROP line like:

```
&PROP ID='Acme Smoke Detector I2',QUANTITY='CHAMBER OBSCURATION',
      ALPHA_E=1.8,BETA_E=-1.1,ALPHA_C=1.0,BETA_C=-0.8,ACTIVATION_OBSCURATION=3.28 /
```

where the two characteristic filling or "lag" times are of the form:

$$\delta t_e = \alpha_e u^{\beta_e} \quad ; \quad \delta t_c = \alpha_c u^{\beta_c} \tag{13.1}$$

The default detector parameters are for the Heskestad model with a characteristic LENGTH of 1.8 m. For the Cleary model, the ALPHAs and BETAs must all be listed explicitly. Suggested constants for unidentified ionization and photoelectric detectors presented in Table 13.1. ACTIVATION_OBSCURATION is the threshold value in units of %/m. The threshold can be set according to the setting commonly provided by the manufacturer. The default setting is 3.28 %/m (1 %/ft).

Table 13.1: Suggested Values for Smoke Detector Model. See Ref. [9] for others.

Detector	α_e	β_e	α_c, L	β_c
Cleary Ionization I1	2.5	-0.7	0.8	-0.9
Cleary Ionization I2	1.8	-1.1	1.0	-0.8
Cleary Photoelectric P1	1.8	-1.0	1.0	-0.8
Cleary Photoelectric P2	1.8	-0.8	0.8	-0.8
Heskestad Ionization	—	—	1.8	—

Defining Smoke

By default, FDS assumes that the smoke from a fire is generated in direct proportion to the heat release rate. A value of `SOOT_YIELD=0.01` on the `REAC` line means that the smoke generation rate is 0.01 of the fuel burning rate. The "smoke" in this case is not explicitly tracked by FDS, but rather is assumed to be a function of the mixture fraction.

Suppose, however, that you want to define your own "smoke" and that you want to specify its production rate independently of the HRR (or even in lieu of an actual fire, like a smouldering source). You might also want to define a mass extinction coefficient for the smoke and an assumed molecular weight (as it will be tracked like a gas species). Finally, you also want to visualize the smoke using the "SMOKE3D" feature in Smokeview. Use the following lines:

```
&SPEC ID='MY SMOKE', MW=29., MASS_EXTINCTION_COEFFICIENT=8700. /
&SURF ID='SMOULDER', TMP_FRONT=1000., MASS_FLUX(1)=0.0001, COLOR='RED' /
&VENT XB=0.6,1.0,0.3,0.7,0.0,0.0, SURF_ID='SMOULDER' /

&PROP ID='Acme Smoke', QUANTITY='CHAMBER OBSCURATION', SPEC_ID='MY SMOKE' /
&DEVC XYZ=1.00,0.50,0.95, PROP_ID='Acme Smoke', ID='smoke_1' /

&DUMP SMOKE3D_QUANTITY='MY SMOKE', DT_PL3D=30. /
```

The same smoke detector model is used that was described above. Only now, the mass fraction of your species `'MY SMOKE'` is used in the algorithm, rather than that associated with the mixture fraction. Note that your species will not participate in the radiation calculation. It will merely serve as a surrogate for smoke. Note also that if you specify explicitly a smoke surrogate, you should set `SOOT_YIELD=0` on the `REAC` line to prevent FDS from including smoke as a mixture fraction species.

13.3.5 Beam Detection Systems

A beam detector can be defined by specifying the endpoints, `(x1,y1,z1) and (x2,y2,z2)`, of the beam and the total percent obscuration at which the detector activates. The two endpoints must lie in the same mesh. FDS determines which mesh cells lie along the linear path defined by the two endpoints. The beam detector response is evaluated as

$$\text{Obscuration} = \left(1 - \exp\left(-K_m \sum_{i=1}^{N} \rho_{soot,i} \, \Delta x_i \right) \right) \times 100 \ \% \tag{13.2}$$

where i is a mesh cell along the path of the beam, $\rho_{soot,i}$ is the soot density of the mesh cell, Δx_i is the distance within the mesh cell that is traversed by the beam, and K_m is the mass extinction coefficient. The line in the input file has the form:

```
&DEVC XB=x1,x2,y1,y2,z1,z2, QUANTITY='PATH OBSCURATION', ID='beam1', SETPOINT=0.33 /
```

Since a single linear path cannot span more than one mesh, having a beam detector that crosses multiple meshes will require post processing. Break the beam detector path into multiple DEVC lines, one for each mesh that the beam crosses. The total obscuration is given by

$$\text{Obscuration} = \left[1 - \prod_{i=1}^{N} (1 - output_i/100) \right] \times 100 \quad \% \tag{13.3}$$

where $output_i$ is the FDS output for the beam detector of the ith path and the symbol, $\prod$, indicates a product rather than a sum.

Example Case: beam_detector

A 10 m by 10 m by 4 m compartment is filled with smoke, represented as 0.006 kg/kg of the mixture fraction species variable, MIXTURE_FRACTION_2[2]. The default soot yield is 0.01 kg/kg, resulting in a uniform soot density of 71.9 mg/m^3. Using the default mass extinction coefficient of 8700 m^2/kg, the optical depth is calculated to be 0.626 m^{-1}. The compartment has a series of obstructions located at increasing distance from the front in increments of 1 m. The correlation for the output quantity VISIBILITY, Eq. (14.9), produces a visibility distance of 4.8 m. When viewing the smoke levels with Smokeview, you should just barely see the fifth obstacle which is at a distance of 5 m from the front of the compartment. If this is the case, Smokeview is properly displaying the obscuration of the smoke. Three beam detectors are also placed in the compartment. These all have a path length of 10 m, but are at different orientations within the compartment. Using the optical depth of 0.626 m^{-1} and the path length of 10 m, the expected total obscuration is 99.81 %, which is the result computed by FDS for each of the three detectors.
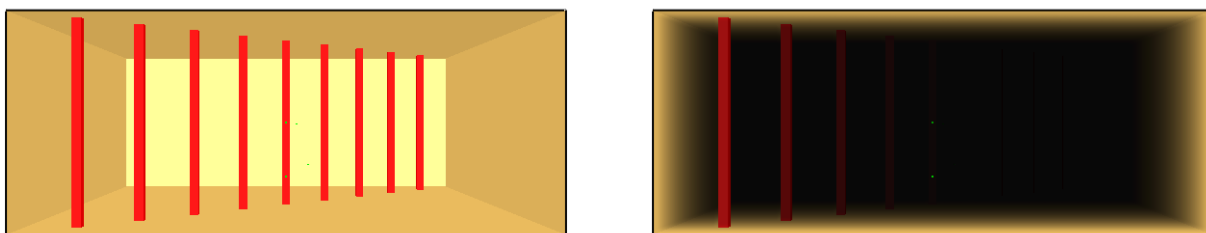
Figure 13.1: Output of the **beam_detector** test case.

13.3.6 Aspiration Detection Systems

An aspiration detection system groups together a series of soot measurement devices. An aspiration system consists of a sampling pipe network that draws air from a series of locations to a central point where an obscuration measurement is made. To define such a system in FDS, you must provide the sampling locations, sampling flow rates, the transport time from each sampling location, and if an alarm output is desired, the overall obscuration "setpoint." One or more DEVC inputs are used to specify details of the sampling locations, and one additional input is used to specify the central detector:

---

[2]In its default mode, the mixture fraction combustion model requires transport equations for two gas species – MIXTURE_FRACTION_1 and MIXTURE_FRACTION_2. The first is just the fuel gas, the second is a combination of the products of combustion.

```
&DEVC XYZ=..., QUANTITY='DENSITY', SPEC_ID='soot', ID='soot1', DEVC_ID='asp1',
      FLOWRATE=0.1, DELAY=20 /
&DEVC XYZ=..., QUANTITY='DENSITY', SPEC_ID='soot', ID='soot2', DEVC_ID='asp1',
      FLOWRATE=0.2, DELAY=10 /
 ...
&DEVC XYZ=..., QUANTITY='DENSITY', SPEC_ID='soot', ID='sootN', DEVC_ID='asp1',
      FLOWRATE=0.3, DELAY=30 /

&DEVC XYZ=..., QUANTITY='ASPIRATION', ID='asp1', BYPASS_FLOWRATE=0.4, SETPOINT=0.02 /
```

where the DEVC_ID is used at each sampling point to reference the central detector, FLOWRATE is the gas flow rate in kg/s, DELAY is the transport time (in seconds) from the sampling location to the central detector, BYPASS_FLOWRATE is the flow rate in kg/s of any air drawn into the system from outside the computational domain (accounts for portions of the sampling network lying outside the domain defined by the MESH inputs), and SETPOINT is the alarm threshold obscuration in units of %/m. The output of the aspiration system is computed as

$$\text{Obscuration} = \left(1 - \exp\left(-K_m \frac{\sum_{i=1}^{N} \rho_{soot,i}(t - t_{d,i}) \, \dot{m}_i}{\sum_{i=1}^{N} \dot{m}_i} \right) \right) \times 100 \ \%/\text{m} \tag{13.4}$$

where $\dot{m}_i$ is the mass FLOWRATE of the ith sampling location, $\rho_{soot,i}(t - t_{d,i})$ is the soot density at the ith sampling location $t_{d,i}$ s prior (DELAY) to the current time t, and K_m is the MASS_EXTINCTION_COEFFICIENT associated with visible light.

Example Case: aspiration_detector

A cubical compartment, 2 m on a side has a three sampling location aspiration system. The three locations have equal flow rates of 0.3 kg/s, and transport times of 50, 100, and 150 s, respectively. No bypass flow rate is specified for the aspiration detector. Combustion products are forced into the bottom of the compartment at a rate of 1 kg/s. The SOOT_YIELD=0.001. Mass is removed from the top of the compartment at a rate of 1 kg/s. The aspiration detector shows an increasing obscuration over time. There is a delay of slightly over 50 s in the initial increase which results from the 50 s transport time for the first sampling location plus a short period of time to transport the combustion products to the sampling location. The detector response has three plateaus that result from the delay times of the sampling locations. The sampling points are co-located, so each plateau represents an additional one third of the soot being transported to the detector. The soot density at the sampling point is 3.493×10^{-4} kg/m^3. Using this value the plateaus are computed as 63.7 %, 86.8 %, and 95.2 %, as seen in Fig. 13.2.

13.3.7 Electrical Cable Failure

Petra Andersson and Patrick Van Hees of the Swedish National Testing and Research Institute (SP) have proposed that the thermally-induced electrical failure (THIEF) of a cable can be predicted via a simple one-dimensional heat transfer calculation, under the assumption that the cable can be treated as a homogenous cylinder [10]. Their results for PVC cables were encouraging and suggested that the simplification of the analysis is reasonable and that it should extend to other types of cables. The assumptions underlying the THIEF model are as follows:

1. The heat penetration into a cable of circular cross section is largely in the radial direction. This greatly simplifies the analysis, and it is also conservative because it is assumed that the cable is completely surrounded by the heat source.

2. The cable is homogenous in composition. In reality, a cable is constructed of several different types of polymeric materials, cellulosic fillers, and a conducting metal, most often copper.
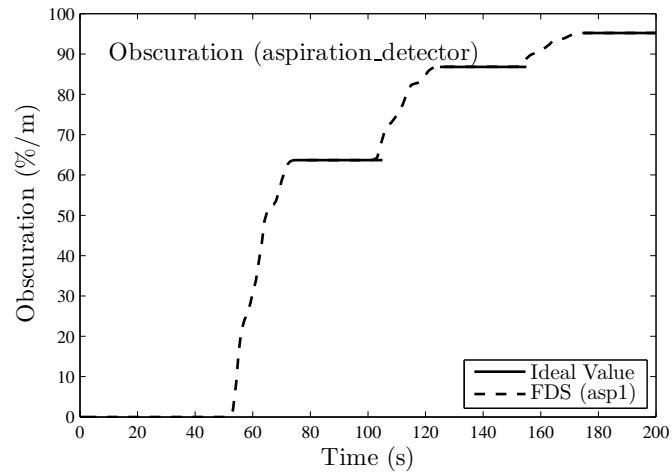
Figure 13.2: Output of **aspiration_detector** test case.

3. The thermal properties – conductivity, specific heat, and density – of the assumed homogenous cable are independent of temperature. In reality, both the thermal conductivity and specific heat of polymers are temperature-dependent, but this information is very difficult to obtain from manufacturers.

4. It is assumed that no decomposition reactions occur within the cable during its heating, and ignition and burning are not considered in the model. In fact, thermoplastic cables melt, thermosets form a char layer, and both off-gas volatiles up to and beyond the point of electrical failure.

5. Electrical failure occurs when the temperature just inside the cable jacket reaches an experimentally determined value.

Obviously, there are considerable assumptions inherent in the Andersson and Van Hees THIEF model, but their results for various polyvinyl chloride (PVC) cables suggested that it may be sufficient for engineering analyses of a wider variety of cables. The U.S. Nuclear Regulatory Commission sponsored a study of cable failure known as CAROLFIRE [11]. The primary project objective of CAROLFIRE was to characterize the various modes of electrical failure (*e.g.* hot shorts, shorts to ground) within bundles of power, control and instrument cables. A secondary objective of the project was to develop a simple model to predict thermally-induced electrical failure when a given interior region of the cable reaches an empirically determined threshold temperature. The measurements used for these purposes are described in Volume II of the CAROLFIRE test report. Volume III describes the modeling.

The THIEF model can only predict the temperature profile within the cable as a function of time, given a time-dependent exposing temperature or heat flux. The model does not predict at what temperature the cable fails electrically. This information is gathered from experiment. The CAROLFIRE experimental program included bench-scale, single cable experiments in which temperature measurements were made on the surface of, and at various points within, cables subjected to a uniform heat flux. These experiments provided the link between internal cable temperature and electrical failure. The model can only predict the interior temperature and infer electrical failure when a given temperature is reached. It is presumed that the temperature of the centermost point in the cable is not necessarily the indicator of electrical failure. This

analysis method uses the temperature just inside the cable jacket rather than the centermost temperature, as that is where electrical shorts in a multi-conductor cable are most likely to occur first.

To use the THIEF model in FDS, add lines similar to the following to the input file:

```
&PROP ID='Acme Cable', QUANTITY='CABLE TEMPERATURE', CABLE_MASS_PER_LENGTH=0.529,
      CABLE_FAILURE_TEMPERATURE=400., CABLE_DIAMETER=0.0163,
      CABLE_JACKET_THICKNESS=0.00152 /
&DEVC XYZ=..., ID='Cable 1', PROP_ID='Acme Cable', ORIENTATION=0,0,1 /
&DEVC XYZ=..., ID='Cable 2', PROP_ID='Acme Cable', ORIENTATION=1,0,1 /
                                   .
                                   .
```

Most of the terms are self-explanatory, and the logic is similar to that of a sprinkler. The THIEF model is invoked by the specific use of the QUANTITY='CABLE TEMPERATURE'. The cable mass per unit length is in units of kg/m, failure temperature in °C, diameter in m, jacket thickness in m. Note that you can use any orientation, rather than just the 6 coordinate directions.

13.4 Basic Control Logic

Devices can be used to control various actions, like creating and removing obstructions, or activating and deactivating fans and vents. Every device has an associated QUANTITY, whether it is included directly on the DEVC line or indirectly on the optional PROP line. Using the DEVC parameter SETPOINT, you can trigger an action to occur when the QUANTITY value passes above, or below, the given SETPOINT. The choice is dictated by the given TRIP_DIRECTION, which is just a positive or negative integer. The following parameters dictate how a device will control something:

SETPOINT The value of the device at which its state changes. For a detection type of device (e.g. heat or smoke) this value is taken from the device's PROP inputs and need not be specified on the DEVC line.

TRIP_DIRECTION A positive integer means the device will change state when its value increases past the setpoint and a negative integer means the device will change state when its value decreases past the setpoint. The default value is +1.

LATCH If this logical value is set to .TRUE. the device will only change state once. The default value is .TRUE..

INITIAL_STATE This logical value is the initial state of the device. The default value is .FALSE. For example, if an obstruction associated with the device is to disappear, set INITIAL_STATE=.TRUE.

If you desire to control FDS using more complex logic than can be provided by the use of a single device and its setpoint, control functions can be specified using the CTRL input. See Section 13.5 for more on CTRL functions. The simplest example of a device is just a timer:

```
&DEVC XYZ=1.2,3.4,5.6, ID='my clock', QUANTITY='TIME', SETPOINT=30. /
```

Anything associated with the device via the parameter, DEVC_ID='my clock', will change its state at 30 s. For example, if the text were added to an OBST line, that obstruction would change from its INITIAL_STATE of .FALSE. to .TRUE. after 30 s. In other words, it would be created at 30 s instead of at the start of the simulation. This is a simple way to open a door or window.

13.4.1 Creating and Removing Obstructions

In many fire scenarios, the opening or closing of a door or window can lead to dramatic changes in the course of the fire. Sometimes these actions are taken intentionally, sometimes as a result of the fire. Within the framework of an FDS calculation, these actions are represented by the creation or removal of solid obstacles, or the opening or closing of exterior vents.

Remove or create a solid obstruction by assigning the character string DEVC_ID the name of a DEVC ID on the OBST line that is to be created or removed. This will direct FDS to remove or create the obstruction when the device changes state to .FALSE. or .TRUE., respectively. For example, the lines

```
&OBST XB=..., SURF_ID='...', DEVC_ID='det2' /
                       .
                       .
&DEVC XYZ=..., PROP_ID='...', ID='det1' /
&DEVC XYZ=..., PROP_ID='...', ID='det2', INITIAL_STATE=.TRUE. /
```

will cause the given obstruction to be removed when the specified DEVC changes state.

Creation or removal at a predetermined time can be performed using a DEVC that has TIME as its measured quantity. For example, the following instructions will cause the specified HOLEs and OBSTstructions to appear/disappear at the various designated times. These lines are part of the simple test case called **create_remove.fds**.

```
&HOLE XB=0.25,0.45,0.20,0.30,0.20,0.30, COLOR='RED',   DEVC_ID='timer 1' /
&HOLE XB=0.25,0.45,0.70,0.80,0.70,0.80, COLOR='GREEN', DEVC_ID='timer 2' /
&OBST XB=0.70,0.80,0.20,0.30,0.20,0.30, COLOR='BLUE',  DEVC_ID='timer 3' /
&OBST XB=0.70,0.80,0.60,0.70,0.60,0.70, COLOR='PINK',  DEVC_ID='timer 4' /

&DEVC XYZ=..., ID='timer 1', SETPOINT= 1., QUANTITY='TIME', INITIAL_STATE=.FALSE./
&DEVC XYZ=..., ID='timer 2', SETPOINT= 2., QUANTITY='TIME', INITIAL_STATE=.TRUE. /
&DEVC XYZ=..., ID='timer 3', SETPOINT= 3., QUANTITY='TIME', INITIAL_STATE=.FALSE./
&DEVC XYZ=..., ID='timer 4', SETPOINT= 4., QUANTITY='TIME', INITIAL_STATE=.TRUE. /
```

The blue obstruction appears at 3 s because its initial state is false, meaning that it does not exist initially. The pink obstruction disappears at 4 s because it does exist initially. The red hole is created at 1 s because it does not exist initially (it is filled in with a red obstruction). The green hole is filled in at 2 s because it does exist (as a hole) initially. **You should always try a simple example first before embarking on a complicated creation/removal scheme for obstructions and holes.**

To learn how to create and remove obstructions multiple times, see Section 13.5.5 for information about the custom control feature.

Starting with FDS version 5.3.0, an obstruction that makes up the boundary of a "pressure zone" (see Section 9.6) *can* be created or removed. The reason for this restriction prior to 5.3 was that abrupt changes in pressure could cause numerical instabilities.

13.4.2 Activating and Deactivating Vents

When a device or control function is applied to a VENT, the purpose is to either activate or deactivate any time ramp associated with the VENT via its SURF_ID. For example, to control a fan with the device 'det2', do the following:

```
&SURF ID='FAN', VOLUME_FLUX=5. /
&VENT XB=..., SURF_ID='FAN', DEVC_ID='det2' /
&DEVC ID='det2', XYZ=..., QUANTITY='TIME', SETPOINT=30., INITIAL_STATE=.FALSE. /
```

Note that at 30 s, the "state" of the 'FAN' changes from .FALSE. to .TRUE., or more simply, the 'FAN' turns on. Since there is no explicit time function associated with the 'FAN', the default 1 s ramp-up will begin at 30 s instead of at 0 s.

If in this example INITIAL_STATE=.TRUE., then the fan should "deactivate," or turn off at 30 s. Essentially, "activation" of a VENT causes all associated time functions to be delayed until the device SETPOINT is reached. "Deactivation" of a VENT turns off all time functions. Usually this means that the parameters on the SURF line are all nullified, so it is a good idea to check the functionality with a simple example.

Until further notice, a 'MIRROR' or 'OPEN' VENT should not be activated or deactivated. You can, however, place an obstruction in front of an 'OPEN' VENT and then create it or remove it to model the closing or opening of a door or window.

13.5   Advanced Control Functions: The `CTRL` Namelist Group

There are many systems whose functionality cannot be described by a simple device with a single "setpoint." Consider for example, a typical HVAC system. It is controlled by a thermostat that is given a temperature setpoint. The system turns on when the temperature goes below the setpoint by some amount and then turns off when the temperature rises above that same setpoint by some amount. This behavior can not be defined by merely specifying a single setpoint. You must also define the range or "deadband" around the setpoint, and whether an increasing or decreasing temperature activates the system. For the HVAC example, crossing the lower edge of the deadband activates heating; crossing the upper edge activates cooling.

While HVAC is not the primary purpose of FDS, there are numerous situations where a system responds to the fire in a non-trivial way. The `CTRL` input is used to define these more complicated behaviors. A control function will take as input the outputs of one or more devices and/or control functions. In this manner, complicated behaviors can be simulated by making functions of other functions. For most of the control function types, the logical value output of the devices and control functions and the time they last changed state are used as the inputs.

For any object for which a `DEVC_ID` can be specified (such as `OBST` or `VENT`), a `CTRL_ID` can be specified instead. A control is identified by the `ID` parameter. The inputs to the control are identified by

Table 13.2: Control function types for `CTRL`

Function Type	Description
ANY	Changes state if any INPUTs are .TRUE.
ALL	Changes state if all INPUTs are .TRUE.
ONLY	Changes state if and only if N INPUTs are .TRUE.
AT_LEAST	Changes state if at least N INPUTs are .TRUE.
TIME_DELAY	Changes state DELAY s after INPUT becomes .TRUE.
CUSTOM	Changes state based on evaluating a RAMP of the function's input
DEADBAND	Behaves like a thermostat
KILL	Terminates code execution if its sole INPUT is .TRUE.
RESTART	Dumps restart files if its sole INPUT is .TRUE.

the `INPUT_ID` parameter. `INPUT_ID` would be passed one or more `ID` strings from either devices or other controls.

If you want to design a system of controls and devices that involves multiple changes of state, include the attribute `LATCH=.FALSE.` on the relevant `DEVC` or `CTRL` input lines. By default, devices and controls may only change state once, like a sprinkler activating or smoke detector alarming. `LATCH=.TRUE.` by default for both devices and controls.

13.5.1   Control Functions: `ANY`, `ALL`, `ONLY`, and `AT_LEAST`

Suppose you want an obstruction to be removed (a door is opened, for example) after any of four smoke detectors in a room has activated. Use input lines of the form:

```
&OBST XB=..., SURF_ID='...', CTRL_ID='SD' /

&DEVC XYZ=1,1,3, PROP_ID='Acme Smoker', ID='SD_1' /
&DEVC XYZ=1,4,3, PROP_ID='Acme Smoker', ID='SD_2' /
```

```
&DEVC XYZ=4,1,3, PROP_ID='Acme Smoker', ID='SD_3' /
&DEVC XYZ=4,4,3, PROP_ID='Acme Smoker', ID='SD_4' /
&CTRL ID='SD', FUNCTION_TYPE='ANY', INPUT_ID='SD_1','SD_2','SD_3','SD_4',
      INITIAL_STATE=.TRUE. /
```

The `INITIAL_STATE` of the control function `SD` is `.TRUE.`, meaning that the obstruction exists initially. The "change of state" means that the obstruction is removed when any smoke detector alarms. By default, the `INITIAL_STATE` of the control function `SD` is `.FALSE.`, meaning that the obstruction does not exist initially.

Suppose that now you want the obstruction to be created (a door is closed, for example) after all four smoke detectors in a room have activated. Use a control line of the form:

```
&CTRL ID='SD', FUNCTION_TYPE='ALL', INPUT_ID='SD_1','SD_2','SD_3','SD_4' /
```

The control functions `AT_LEAST` and `ONLY` are generalizations of `ANY` and `ALL`. For example,

```
&CTRL ID='SD', FUNCTION_TYPE='AT_LEAST', N=3, INPUT_ID='SD_1','SD_2','SD_3','SD_4' /
```

changes the state from `.FALSE.` to `.TRUE.` when at least 3 detectors activate. Note that in this example, and the example below, the parameter `N` is used to specify the number of activated or "TRUE" inputs required for the conditions of the Control Function to be satisfied. The control function,

```
&CTRL ID='SD', FUNCTION_TYPE='ONLY', N=3, INPUT_ID='SD_1','SD_2','SD_3','SD_4' /
```

changes the state from `.FALSE.` to `.TRUE.` when 3, and only 3, detectors activate.

13.5.2   Control Function: `TIME_DELAY`

There is often a time delay between when a device activates and when some other action occurs, like in a dry pipe sprinkler system.

```
&DEVC XYZ=2,2,3, PROP_ID='Acme Sprinkler_link', QUANTITY='LINK TEMPERATURE',
      ID='Spk_29_link', CTRL_ID='dry pipe' /
&DEVC XYZ=2,2,3, PROP_ID='Acme Sprinkler', QUANTITY='CONTROL', ID='Spk_29',
      CTRL_ID='dry pipe' /
&CTRL ID='dry pipe', FUNCTION_TYPE='TIME_DELAY', INPUT_ID='Spk_29_link', DELAY=30. /
```

This relationship between a sprinkler and its pipes means that the sprinkler spray is controlled (in this case delayed) by the `'dry pipe'`, which adds 30 s to the activation time of `Spk_29`, measured by `Spk_29_link`, before water can flow out of the head.

13.5.3   Control Function: `DEADBAND`

This control function behaves like an HVAC thermostat. It can operate in one of two modes analagous to heating or cooling. The function is provided with an `INPUT_ID` which is the `DEVC` whose value is used by the function, a `DEADBAND`, and the mode of operation by `ON_BOUND`. If `ON_BOUND='LOWER'`, the function changes state from its `INITIAL_VALUE` when the value of the `INPUT_ID` drops below the lower value in `DEADBAND` and reverts when it increases past the upper value, i.e. like a heating system. The reverse will occur if `ON_BOUND='UPPER'`, i.e. like a cooling system.

For an HVAC example, the following lines of input would set up a simple thermostat:

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```
&SURF ID='FAN', TMP_FRONT=40., VOLUME_FLUX=-1. /
&VENT XB=-0.3,0.3,-0.3,0.3,0.0,0.0, SURF_ID='FAN', CTRL_ID='thermostat' /
&DEVC ID='TC', XYZ=2.4,5.7,3.6, QUANTITY='TEMPERATURE' /
&CTRL ID='thermostat', FUNCTION_TYPE='DEADBAND', INPUT_ID='TC',
      ON_BOUND='LOWER', SETPOINT=23.,27.,LATCH=.FALSE./
```

Here, we want to control the `VENT` that simulates the `FAN`, which blows hot air into the room. A `DEVC` called `TC` is positioned in the room to measure the `TEMPERATURE`. The `thermostat` uses a `SETPOINT` to turn on the `FAN` when the temperature falls below 23 °C (`ON_BOUND='LOWER'`) and it turns off when the temperature rises above 27 °C.

Note that a deadband controller needs to have `LATCH` set to `.FALSE.`.

13.5.4 Control Function: `RESTART` and `KILL`

There are times when you might only want to run a simulation until some goal is reached. Previously this could generally only be done by constantly monitoring the simulation's output and manually stopping the calculation when you determine that the goal has been reached. The `KILL` control function can do this automatically.

Additionally there are analyses where you might want to create some baseline condition and then run multiple permutations of that baseline. For example, you might want to run a series of simulations where different mitigation strategies are tested once a detector alarms. Using the `RESTART` control function, you can cause a restart file to be created once a desired condition is met. The simulation can continue and the restart files can be copied to have the job identifying string, `CHID`, of the various permutations (providing of course that the usual restrictions on the use of restart files are followed). For example, the lines

```
&DEVC ID='temp', QUANTITY='TEMPERATURE', SETPOINT=1000., XYZ=4.5,6.7,3.6 /
&DEVC ID='velo', QUANTITY='VELOCITY', SETPOINT=10., XYZ=4.5,6.7,3.6 /

&CTRL ID='kill', FUNCTION_TYPE='KILL', INPUT_ID='temp' /
&CTRL ID='restart', FUNCTION_TYPE='RESTART', INPUT_ID='velo' /
```

will "kill" the job and output restart files when the temperature at the given point rises above 1000 °C; or just force restart files to be output when the velocity at a given point exceeds 10 m/s.

13.5.5 Control Function: `CUSTOM`

For most of the control function types, the logical (true/false) output of the devices and control functions and the time they last changed state are taken as inputs. A `CUSTOM` function uses the numerical output of a `DEVC` along with a `RAMP` to determine the output of the function. When the `RAMP` output for the `DEVC` value is negative, the `CTRL` will have the value of its `INITIAL_STATE`. When the `RAMP` output for the `DEVC` value is positive, the `CTRL` will have the opposite value of its `INITIAL_STATE`. In the case below, the `CUSTOM` control function uses the numerical output of a timer device as its input. The function returns true (the default value for `INITIAL_STATE` is `.FALSE.`) when the `F` parameter in the ramp specified with `RAMP_ID` is a positive value and false when the `RAMP` `F` value is negative. In this case, the control would start false and would switch to true when the timer reaches 60 s. It would then stay in a true state until the timer reaches 120 s and would then change back to false.

Note that when using control functions the `ID`s assigned to both the `CTRL` and the `DEVC` inputs must be unique across both sets of inputs, i.e. you cannot use the same `ID` for both a control function and a device.

In the HVAC example above, we could set the system to function on a fixed cycle by using a `CUSTOM` control function based on time:

```
&SURF ID='FAN', TMP_FRONT=40., VOLUME_FLUX=-1. /
&VENT XB=-0.3,0.3,-0.3,0.3,0.0,0.0, SURF_ID='FAN', CTRL_ID='cycling timer' /
&DEVC ID='TIMER', XYZ=2.4,5.7,3.6, QUANTITY='TIME' /
&CTRL ID='cycling timer', FUNCTION_TYPE='CUSTOM, INPUT_ID='TIMER', RAMP_ID='cycle' /
&RAMP ID='cycle', T= 59, F=-1 /
&RAMP ID='cycle', T= 61, F= 1 /
&RAMP ID='cycle', T=119, F= 1 /
&RAMP ID='cycle', T=121, F=-1 /
```

In the above example the fan will be off initially, turn on at 60 s and then turn off at 120 s.

You can make an obstruction appear and disappear multiple times by using lines like

```
&OBST XB=..., SURF_ID='whatever', CTRL_ID='cycling timer' /
&DEVC ID='TIMER', XYZ=..., QUANTITY='TIME' /
&CTRL ID='cycling timer', FUNCTION_TYPE='CUSTOM', INPUT_ID='TIMER', RAMP_ID='cycle' /
&RAMP ID='cycle', T=  0, F=-1 /
&RAMP ID='cycle', T= 59, F=-1 /
&RAMP ID='cycle', T= 61, F= 1 /
&RAMP ID='cycle', T=119, F= 1 /
&RAMP ID='cycle', T=121, F=-1 /
```

The above will have the obstacle initially removed, then added at 60 s, and removed again at 120 s.

Experiment with these combinations using a simple case before trying a case to make sure that FDS indeed is doing what is intended.

13.5.6 Combining Control Functions: A Pre-Action Sprinkler System

For a pre-action sprinkler system, the normally dry sprinkler pipes are flooded when a detection event occurs. For this example, the detection event is when two of four smoke detectors alarm. It takes 30 s to flood the piping network. The nozzle is a `DEVC` named 'NOZZLE 1' controlled by the `CTRL` named 'nozzle trigger'. The nozzle activates when both detection <u>and</u> the time delay have occurred. Note that the `DEVC` is specified with `QUANTITY='CONTROL'`.

```
&DEVC XYZ=1,1,3, PROP_ID='Acme Smoker', ID='SD_1' /
&DEVC XYZ=1,4,3, PROP_ID='Acme Smoker', ID='SD_2' /
&DEVC XYZ=4,1,3, PROP_ID='Acme Smoker', ID='SD_3' /
&DEVC XYZ=4,4,3, PROP_ID='Acme Smoker', ID='SD_4' /
&DEVC XYZ=2,2,3, PROP_ID='Acme Nozzle', QUANTITY='CONTROL',
      ID='NOZZLE 1', CTRL_ID='nozzle trigger' /

&CTRL ID='nozzle trigger', FUNCTION_TYPE='ALL', INPUT_ID='smokey','delay' /
&CTRL ID='delay', FUNCTION_TYPE='TIME_DELAY', INPUT_ID='smokey', DELAY=30. /
&CTRL ID='smokey', FUNCTION_TYPE='AT_LEAST', N=2, INPUT_ID='SD_1','SD_2','SD_3','SD_4' /
```

13.5.7 Combining Control Functions: A Dry Pipe Sprinkler System

For a dry-pipe sprinkler system, the normally dry sprinkler pipes are pressurized with gas. When a link activates in a sprinkler head, the pressure drop allows water to flow into the pipe network. For this example it takes 30 s to flood the piping network once a sprinkler link has activated. The sequence of events required for operation is first `ANY` of the links must activate which starts the 30 s `TIME_DELAY`. Once the 30 s delay has occurred, each nozzle with an active link, the `ALL` control functions, will then flow water.

```
&DEVC XYZ=2,2,3, PROP_ID='Acme Sprinkler Link', ID='LINK 1' /
&DEVC XYZ=2,3,3, PROP_ID='Acme Sprinkler Link', ID='LINK 2' /

&PROP ID='Acme Sprinkler Link', QUANTITY='LINK TEMPERATURE',
      ACTIVATION_TEMPERATURE=74., RTI=30./

&DEVC XYZ=2,2,3, PROP_ID='Acme Nozzle', QUANTITY='CONTROL',
      ID='NOZZLE 1', CTRL_ID='nozzle 1 trigger' /
&DEVC XYZ=2,3,3, PROP_ID='Acme Nozzle', QUANTITY='CONTROL',
      ID='NOZZLE 2', CTRL_ID='nozzle 2 trigger' /

&CTRL ID='check links', FUNCTION_TYPE='ANY', INPUT_ID='LINK 1','LINK 2'/
&CTRL ID='delay', FUNCTION_TYPE='TIME_DELAY', INPUT_ID='check links', DELAY=30. /
&CTRL ID='nozzle 1 trigger', FUNCTION_TYPE='ALL', INPUT_ID='delay','LINK 1'/
&CTRL ID='nozzle 2 trigger', FUNCTION_TYPE='ALL', INPUT_ID='delay','LINK 2'/
```

Chapter 14

Output Data

Before a calculation is started, carefully consider what information should be saved. All output quantities must be specified at the start of the calculation. In most cases, there is no way to retrieve information after the calculation ends if it was not specified from the start. There are several different ways of visualizing the results of a calculation. Most familiar to experimentalists is to save a given quantity at a single point in space so that this quantity can be plotted as a function of time, like a thermocouple temperature measurement. The namelist group DEVC, described previously, is used to specify point measurements.

To visualize the flow patterns better, save planar slices of data, either in the gas or solid phases, by using the SLCF (SLiCe File) or BNDF (BouNDary File) namelist group. Both of these output formats permit you to animate these quantities in time.

For static pictures of the flow field, use the PLot3D files that are automatically generated 5 times a run. Plot3D format is used by many CFD programs as a simple way to store specified quantities over the entire mesh at one instant in time.

Finally, tracer particles can be injected into the flow field from vents or obstacles, and then viewed in Smokeview. Use the PART namelist group to control the injection rate, sampling rate and other parameters associated with particles.

Note: unlike in FDS version 1, particles are no longer used to introduce heat into the flow, thus particles no longer are ejected automatically from burning surfaces.

14.1 Output Control Parameters: The DUMP Namelist Group

The namelist group DUMP contains parameters (Table 15.5) that control the rate at which output files are written, and various other global parameters associated with output files. This namelist group is new starting in FDS 5, although its parameters have been specified via other namelist groups in past versions.

NFRAMES Number of output dumps per calculation. The default is 1000. Device data, slice data, particle data, isosurface data, 3D smoke data, boundary data, solid phase profile data, and control function data are saved every (T_END-T_BEGIN)/NFRAMES seconds unless otherwise specified using DT_DEVC, DT_SLCF, DT_PART, DT_ISOF, DT_BNDF, DT_PROF, or DT_CTRL Note that DT_SLCF controls Smoke3D output. DT_HRR controls the output of heat release rate and associated quantities.

MASS_FILE If .TRUE., produce an output file listing the total masses of all gas species as a function of time. It is .FALSE. by default because the calculation of all gas species in all mesh cells is time-consuming. The parameter DT_MASS controls the frequency of output.

STATE_FILE If .TRUE., produce an output file listing the species mass fractions associated with the mixture fraction, assuming complete combustion. It is .FALSE. by default, and only makes sense for calculations involving the mixture fraction model.

MAXIMUM_DROPLETS Maximum number of Lagrangian particles that can be included on any mesh at any given time. (Default 500000)

SMOKE3D If .FALSE., do not produce an animation of the smoke and fire. It is .TRUE. by default.

FLUSH_FILE_BUFFERS FDS purges the output file buffers periodically and forces the data to be written out into the respective output files. It does this to make it easier to view the case in Smokeview while it is running. It has been noticed on Windows machines that occasionally a runtime error occurs because of file access problems related to the buffer flushing. If this happens, set this parameter to .FALSE., but be aware that it may not be possible to look at output in Smokeview until after the calculation is finished. You may also set DT_FLUSH to control the frequency of the file flushing. Its default value is the duration of the simulation divided by NFRAMES.

STATUS_FILES If .TRUE., produces an output file **CHID.notready** which is deleted, if the simulation is completed successfully. This file can be used as an error indicator. It is .FALSE. by default.

14.2 Output File Types

FDS has various types of output files that store computed data. Some of the files are in binary format and intended to be read and rendered by Smokeview. Some of the files are just comma-delimited text files. It is important to remember that you must explicitly declare in the input file most of the FDS output data. A considerable amount of the input file is usually devoted to this.

14.2.1 Device Output: The DEVC Namelist Group

For many commonly used measurement devices there is no need to associate a specific PROP line to the DEVC entry. In such cases, use the character string QUANTITY to indicate that a particular gas or solid phase quantity at the point should be recorded in the output file with the suffix **_devc.csv**. The quantities are listed in Table 14.1. Many of the gas phase quantities are self-explanatory. For example, if you just want to record the time history of the temperature at a given point, add

```
&DEVC XYZ=6.7,2.9,2.1, QUANTITY='TEMPERATURE', ID='T-1' /
```

and a column will be added to the output file **CHID_devc.csv** under the label 'T-1'. In this case, the ID has no other role than as a column label in the output file. Note that versions of FDS prior to version 5 used an 8 cell linear interpolation for a given *gas phase* point measurement. In other words, if you specified a point via the triplet of real numbers, XYZ, FDS would calculate the value of the quantity by linearly interpolating the values defined at the centers of the 8 nearest cells. Starting in FDS 5, this is no longer done. Instead, FDS reports the value of the QUANTITY in the cell where the point XYZ is located.

When prescribing a solid phase quantity, be sure to position the probe at a solid surface. It is not always obvious where the solid surface is since the mesh does not always align with the input obstruction locations. To help locate the appropriate surface, the parameter IOR *must* be included when designating a solid phase quantity, except when using the STATISTICS feature described in Section 14.3.10 in which case the output quantity is not associated with just a single point on the surface. If the orientation of the solid surface is in the positive *x* direction IOR=1, negative *x* direction IOR=-1, positive *y* IOR=2, negative IOR=-2, positive *z* IOR=3, and negative *z* IOR=-3. There are still instances where FDS cannot determine which solid surface is being designated, in which case an error message appears in the diagnostic output file. Re-position the probe and try again. For example, the line

```
&DEVC XYZ=0.7,0.9,2.1, QUANTITY='WALL TEMPERATURE', IOR=-2, ID='...' /
```

designates the surface temperature of a wall facing the negative *y* direction.

In addition to point measurements, the DEVC group can be used to report integrated quantities (See Table 14.1). For example, you may want to know the mass flow out of a door or window. To report this, add the line

```
&DEVC XB=0.3,0.5,2.1,2.5,3.0,3.0, QUANTITY='MASS FLOW', ID='whatever' /
```

Note that in this case, a plane is specified rather than a point. The sextuplet XB is used for this purpose. Notice when a flow is desired, two of the six coordinates need to be the same. Another QUANTITY, HRR, can be used to compute the total heat release rate within a subset of the domain. In this case, the sextuplet XB ought to define a volume rather than a plane. Specification of the plane or volume over which the integration is to take place can only be done using XB – avoid planes or volumes that cross multiple mesh boundaries. FDS has to decide which mesh to use in the integration, and it chooses the finest mesh overlapping the centroid of the designated plane or volume.

14.2.2 Quantities within Solids: The PROF Namelist Group

FDS uses a fine, non-uniform, one-dimensional mesh at each boundary cell to compute heat transfer within a solid. The parameters (Table 15.16) to specify a given PROFile are similar to those used to specify a surface quantity in the DEVC group. XYZ designates the triplet of coordinates, QUANTITY is the physical quantity to monitor, IOR the orientation, and ID an identifying character string. Here is an example of how you would use this feature to get a time history of temperature profiles within a given solid obstruction:

```
&PROF XYZ=..., QUANTITY='TEMPERATURE', ID='TU1SA_FDS', IOR=3 /
```

Other possible quantities are the total density of the wall (QUANTITY = 'DENSITY') or densities of solid material components (QUANTITY = 'MATL_ID'), where MATL_ID is the name of the material.

Each PROF line creates a separate file. This may be more than is needed. Sometimes, all you want to know is the temperature at a certain depth. To get an inner wall temperature, you can also just use a device as follows:

```
&DEVC XYZ=..., QUANTITY='INSIDE WALL TEMPERATURE', DEPTH=0.005, ID='Temp_1', IOR=3 /
```

The parameter DEPTH (m) indicates the distance inside the solid surface. Note that this QUANTITY is allowed only as a DEVC, not a BNDF, output. Also note that if the wall thickness is decreasing over time due to the solid phase reactions, the distance is measured from the current surface, and the measurement point is 'moving' towards the back side of the solid. Eventually, the measurement point may get out of the solid, in which case it starts to show ambient temperature. If you just want to know the temperature of the back surface of the "wall," then use

```
&DEVC XYZ=..., QUANTITY='BACK WALL TEMPERATURE', ID='Temp_b', IOR=3 /
```

Note that this quantity is only meaningful if the front or exposed surface of the "wall" has the attribute BACKING='EXPOSED' on the SURF line that defines it. The coordinates, XYZ, and orientation, IOR, refer to the front surface. To check that the heat conduction calculation is being done properly, you can add the additional line

```
&DEVC XYZ=..., QUANTITY='WALL TEMPERATURE', ID='Temp_f', IOR=-3 /
```

where now XYZ and IOR refer to the coordinates and orientation of the back side of the wall. These two wall temperatures ought to be the same. Remember that the "wall" in this case can only be at most one mesh cell thick, and its THICKNESS need not be the same as the mesh cell width. Rather, the THICKNESS ought to be the actual thickness of the "wall" through which FDS performs a 1-D heat conduction calculation.

14.2.3 Animated Planar Slices: The SLCF Namelist Group

The SLCF ("slice file") namelist group parameters (Table 15.21) allows you to record various gas phase quantities at more than a single point. A "slice" refers to a subset of the whole domain. It can be a line, plane, or volume, depending on the values of XB. The sextuplet XB indicates the boundaries of the "slice" plane. XB is prescribed as in the OBST or VENT groups, with the possibility that 0, 2, or 4 out of the 6 values be the same to indicate a volume, plane or line, respectively. A handy trick is to specify, for example, PBY=5.3 instead of XB if it is desired that the entire plane $y = 5.3$ slicing through the domain be saved. PBX and PBZ control planes perpendicular to the x and z axes, respectively.

Animated vectors can be created in Smokeview if a given SLCF line has the attribute VECTOR=.TRUE. If two SLCF entries are in the same plane, then only one of the lines needs to have VECTOR=.TRUE. Otherwise, a redundant set of velocity component slices will be created.

Normally, FDS averages slice file data at cell corners. For example, gas temperatures are computed at cell centers, but they are linearly interpolated to cell corners and output to a file that is read by Smokeview. To prevent this from happening, set `CELL_CENTERED=.TRUE.` This forces FDS to output the actual cell-centered data with no averaging. Note that this feature is mainly useful for diagnostics because it enables you to visualize the values that FDS actually computes. Note also that this feature should only be used for scalar quantities that are computed at cell centers, like temperatures, mass fractions, *etc.*

Slice file information is recorded in files (See Section 19.7) labeled **CHID_*n*.sf**, where *n* is the index of the slice file. A short fortran program **fds2ascii.f** produces a text file from a line, plane or volume of data. See Section 14.4 for more details.

14.2.4 Animated Boundary Quantities: The `BNDF` Namelist Group

The `BNDF` ("boundary file") namelist group parameters allows you to record surface quantities at all solid obstructions. As with the `SLCF` group, each quantity is prescribed with a separate `BNDF` line, and the output files are of the form **CHID_*n*.bf**. No physical coordinates need be specified, however, just `QUANTITY`. See Table 14.1. For certain output quantities, additional parameters need to be specified via the `PROP` namelist group. In such cases, add the character string, `PROP_ID`, to the `BNDF` line to tell FDS where to find the necessary extra information.

Note that `BNDF` files (Section 19.9) can become very large, so be careful in prescribing the time interval. One way to reduce the size of the output file is to turn off the drawing of boundary information on desired obstructions. On any given `OBST` line, if the string `BNDF_OBST=.FALSE.` is included, the obstruction is not colored. To turn off all boundary drawing, set `BNDF_DEFAULT=.FALSE.` on the `MISC` line. Then individual obstructions can be turned back on with `BNDF_OBST=.TRUE.` on the appropriate `OBST` line. Individual faces of a given obstruction can be controlled via `BNDF_FACE(IOR)`, where `IOR` is the index of orientation (+1 for the positive *x* direction, -1 for negative, and so on).

Normally, FDS averages boundary file data at cell corners. For example, surface temperatures are computed at the center of each surface cell, but they are linearly interpolated to cell corners and output to a file that is read by Smokeview. To prevent this from happening, set `CELL_CENTERED=.TRUE.` on the `BNDF` line. This forces FDS to output the actual cell-centered data with no averaging. Note that this feature is mainly useful for diagnostics because it enables you to visualize the values that FDS actually computes.

14.2.5 Animated Isosurfaces: The `ISOF` Namelist Group

The `ISOF` ("ISOsurface File") namelist group is used to specify the output of gas phase scalar quantities, as three dimensional animated contours. For example, a 300 °C temperature isosurface shows where the gas temperature is 300 °C. Three different values of the temperature can be saved via the line:

```
&ISOF QUANTITY='TEMPERATURE', VALUE(1)=50., VALUE(2)=200., VALUE(3)=500. /
```

where the values are in degrees C. Note that the isosurface output files **CHID_*n*.iso** can become very large, so experiment with different sampling rates (`DT_ISOF` on the `DUMP` line).

Any gas phase quantity can animated via iso-surfaces, but use caution. To render an iso-surface, the desired quantity must be computed in every mesh cell at every output time step. For quantities like `TEMPERATURE`, this is not a problem, as FDS computes it and saves it anyway. However, `soot density` or `oxygen` demand substantial amounts of time to compute at each mesh cell.

14.2.6 Plot3D Static Data Dumps

By default, flow field data in Plot3D format is output 5 times a run. Five quantities are written out to a file at one instant in time. The default specification is:

```
&DUMP ..., PLOT3D_QUANTITY(1:5)='TEMPERATURE',
       'U-VELOCITY','V-VELOCITY','W-VELOCITY','HRRPUV' /
```

It's best to leave the velocity components as is, because Smokeview uses them to draw velocity vectors. The first and fifth quantities can be changed with the parameters `PLOT3D_QUANTITY(1)` and `PLOT3D_QUANTITY(5)` on the `DUMP` line. If any of the specified quantities require the additional specification of a particular species, use `PLOT3D_SPEC_ID(n)` to provide the `SPEC_ID` for `PLOT3D_QUANTITY(n)`.

Note that there can only be one `DUMP` line.

Data stored in Plot3D [12] files (See Section 19.8) use a format developed by NASA and used by many CFD programs for representing simulation results. Plot3D data is visualized in three ways: as 2D contours, vector plots and iso-surfaces. Vector plots may be viewed if one or more of the *u*, *v* and *w* velocity components are stored in the Plot3D file. The vector length and direction show the direction and relative speed of the fluid flow. The vector colors show a scalar fluid quantity such as temperature. Plot3D data are stored in files with extension `.q` . There is an optional file that can be output with coordinate information if another visualization package is being used to render the files. If you write `WRITE_XYZ=.TRUE.` on the `DUMP` line, a file with suffix `.xyz` is written out. Smokeview does not require this file because the coordinate information can be obtained elsewhere.

14.2.7 SMOKE3D: Realistic Smoke and Fire

When you do a fire simulation using the default mixture fraction combustion model, FDS automatically creates two output files that are rendered by Smokeview as realistic looking smoke and fire. By default, the output quantities are the 'MASS FRACTION' of 'soot' and 'HRRPUV' (Heat Release Rate Per Unit Volume) are used in the visualization. You have the option of rendering any other species mass fraction instead of 'soot', so long as the `MASS_EXTINCTION_COEFFICIENT` (either from the `REAC` line, or over-ridden by the value on the `SPEC` line) is appropriate in describing the attenuation of visible light by the specified gas species. The alternative gas species is given by `SMOKE3D_QUANTITY` on the `DUMP` line. If the specified quantity requires the additional specification of a particular species, use `SMOKE3D_SPEC_ID` to provide the `SPEC_ID`. See the Smokeview User's Guide for more details on how these quantities are rendered.

Here is an example of how to control the smoke species. Normally, you do not need to do this as the "smoke" is an assumed part of the default mixture fraction model.

```
&SPEC ID='MY SMOKE', MW=29., MASS_EXTINCTION_COEFFICIENT=8700. /
&SURF ID='NO FIRE', TMP_FRONT=1000., MASS_FLUX(1)=0.0001, COLOR='RED' /
&VENT XB=0.6,1.0,0.3,0.7,0.0,0.0, SURF_ID='NO FIRE' /
&DUMP SMOKE3D_QUANTITY='MASS FRACTION', SMOKE3D_SPEC_ID='MY SMOKE' /
```

The production rate of 'MY SMOKE' is 0.0001 kg/m^2/s, applied to an area of 0.16 m^2. The `MASS_EXTINCTION_COEFFICIENT` is passed to Smokeview to be used for visualization.

14.3 Special Output Quantities

This section lists a variety of output quantities that are useful for studying thermally-driven flows, combustion, pyrolysis, and so forth. Note that some of the output quantities can be produced in a variety of ways.

14.3.1 Heat Release Rate

Quantities associated with the overall energy budget are reported in the comma delimited file **CHID_hrr.csv**. This file is automatically generated; the only input parameter associated with it is `DT_HRR` on the `DUMP` line. The file consists of six columns. The first column contains the time in seconds. The second through fifth columns contain integrated energy gains and losses, all in units of kW. The second column contains the total heat release rate, the third contains the radiative heat loss to all the boundaries (solid and open), the fourth contains the convective and radiative heat loss to the boundaries (*i.e.* the energy flowing out of or into the domain), and the fifth contains the energy conducted into the solid surfaces. The sixth column contains the total burning rate of fuel, in units of kg/s. It is included merely as a check of the total heat release rate.

Let Ω denote the unblocked computational domain, *i.e.* the volume within the bounding rectangle occupied by gas. Let $\partial\Omega$ by the boundary of Ω. The boundary can be divided into two parts $\partial\Omega = \partial\Omega_1 + \partial\Omega_2$. The first part $\partial\Omega_1$ consists of all the solid walls. The second part $\partial\Omega_2$ consists of openings from outside the domain through which gases may flow. This could be an open window to the exterior, or a forced vent.

The total heat release rate is given by

$$\dot{Q} = \int_\Omega \dot{q}''' \, dV \tag{14.1}$$

The radiative loss to the boundaries can be computed with either a volume or boundary integral

$$\dot{Q}_r = \int_\Omega \nabla \cdot \mathbf{q}_r \, dV = \int_{\partial\Omega} \mathbf{q}_r \cdot d\mathbf{S} = \int_{\partial\Omega} \dot{q}_r'' \, dA \tag{14.2}$$

It represents the energy radiating away from the fire and hot gases into the solid boundaries or out of the computational domain. The convective/radiative loss to open boundaries is

$$\dot{Q}_{conv} = \int_{\partial\Omega} c_p \, \rho \, (T - T_\infty) \, \mathbf{u} \cdot d\mathbf{S} + \int_{\partial\Omega_2} \dot{q}_r'' \, dA \tag{14.3}$$

where the integral is positive if the flow and radiative flux are going out of the domain. The conductive loss to solid surfaces is given by

$$\dot{Q}_{cond} = \int_{\partial\Omega_1} \dot{q}_r'' + \dot{q}_c'' \, dA \tag{14.4}$$

where the integral is positive if heat is being lost into a wall colder than the gas.

For scenarios in which the fire is the primary source of energy, after the gas temperatures within the computational domain reach a nearly steady state

$$\dot{Q} \approx \dot{Q}_{conv} + \dot{Q}_{cond} \tag{14.5}$$

This is merely a check of the global energy balance, that is, the energy generated within the space heats up the gases and solid surfaces, and then a balance between heat input and output is achieved.

Note that, in axially symmetric simulations, the volume Ω is the volume of the cylindrical sector

$$\Omega = \frac{1}{2} \left(\texttt{XB(2)} - \texttt{XB(1)} \right)^2 \left(\texttt{XB(4)} - \texttt{XB(3)} \right) \left(\texttt{XB(6)} - \texttt{XB(5)} \right) \tag{14.6}$$

14.3.2 Visibility and Obscuration

If you are performing a fire calculation using the mixture fraction approach, the smoke is tracked along with all other major products of combustion. The most useful quantity for assessing visibility in a space is the *light extinction coefficient*, K [13]. The intensity of monochromatic light passing a distance L through smoke is attenuated according to

$$I/I_0 = e^{-KL} \tag{14.7}$$

The light extinction coefficient, K, is a product of the density of smoke particulate, ρY_s, and a mass specific extinction coefficient that is fuel dependent

$$K = K_m \, \rho Y_s \tag{14.8}$$

Devices that output a % obscuration such as a `DEVC` with a `QUANTITY` of `ASPIRATION`, `CHAMBER OBSCURATION` (smoke detector), or `PATH OBSCURATION` (beam detector) are discussed respectively in Section 13.3.6, Section 13.3.4, and Section 13.3.5

Estimates of visibility through smoke can be made by using the equation

$$S = C/K \tag{14.9}$$

where C is a non-dimensional constant characteristic of the type of object being viewed through the smoke, *i.e.* $C = 8$ for a light-emitting sign and $C = 3$ for a light-reflecting sign [13]. Since K varies from point to point in the domain, the visibility S does as well. Keep in mind that FDS can only track smoke whose production rate and composition are specified. Predicting either is beyond the capability of the present version of the model.

Three parameter control smoke production and visibility; each parameter is input on the `REAC` line. The first parameter is `SOOT_YIELD`, which is the fraction of fuel mass that is converted to soot if the mixture fraction model is being used. The second parameter is called the `MASS_EXTINCTION_COEFFICIENT`, and it is the K_m in Eq. (14.8). The default value is 8700 m^2/kg, a value suggested for flaming combustion of wood and plastics[1]. The third parameter is called the `VISIBILITY_FACTOR`, the constant C in Eq. (14.9). It is 3 by default.

The gas phase output quantity `'EXTINCTION COEFFICIENT'` is K. A similar quantity is the `'OPTICAL DENSITY'`, $K/2.3$, the result of using $\log_{10}$ in the definition

$$D \equiv -\frac{1}{L} \log_{10}\left(\frac{I}{I_0}\right) = K \log_{10} e \tag{14.10}$$

The visibility S is output via the keyword `VISIBILITY`. Note that, by default, the visibility is associated with the smoke that is implicitly defined by the mixture fraction model. However, this quantity can also be associated with an explicitly defined species via the inclusion of a `SPEC_ID`. In other words, you can specify the output quantity `'VISIBILITY'` along with a `SPEC_ID`. This does not require that you do a mixture fraction calculation; only that you have specified the given species via a separate `SPEC` line. You can specify a unique `MASS_EXTINCTION_COEFFICIENT` on the `SPEC` line as well.

14.3.3 Layer Height and the Average Upper and Lower Layer Temperatures

Fire protection engineers often need to estimate the location of the interface between the hot, smoke-laden upper layer and the cooler lower layer in a burning compartment. Relatively simple fire models, often referred to as *two-zone models*, compute this quantity directly, along with the average temperature of the upper

---

[1]For most flaming fuels, a suggested value for K_m is 8700 m^2/kg $\pm$ 1100 m^2/kg at a wavelength of 633 nm [14]

and lower layers. In a computational fluid dynamics (CFD) model like FDS, there are not two distinct zones, but rather a continuous profile of temperature. Nevertheless, there are methods that have been developed to estimate layer height and average temperatures from a continuous vertical profile of temperature. One such method [15] is as follows: Consider a continuous function $T(z)$ defining temperature T as a function of height above the floor z, where $z = 0$ is the floor and $z = H$ is the ceiling. Define T_u as the upper layer temperature, T_l as the lower layer temperature, and z_{int} as the interface height. Compute the quantities:

$$(H - z_{int})\, T_u + z_{int}\, T_l = \int_0^H T(z)\, dz \;\; = \;\; I_1$$

$$(H - z_{int})\, \frac{1}{T_u} + z_{int}\, \frac{1}{T_l} = \int_0^H \frac{1}{T(z)}\, dz \;\; = \;\; I_2$$

Solve for z_{int}:

$$z_{int} = \frac{T_l(I_1 I_2 - H^2)}{I_1 + I_2 T_l^2 - 2 T_l H} \tag{14.11}$$

Let T_l be the temperature in the lowest mesh cell and, using Simpson's Rule, perform the numerical integration of I_1 and I_2. T_u is defined as the average upper layer temperature via

$$(H - z_{int})\, T_u = \int_{z_{int}}^H T(z)\, dz \tag{14.12}$$

Further discussion of similar procedures can be found in Ref. [16].

The quantities LAYER HEIGHT, UPPER TEMPERATURE and LOWER TEMPERATURE can be designated via "device" (DEVC) lines in the input file[2]. For example, the entry

```
&DEVC XB=2.0,2.0,3.0,3.0,0.0,3.0, QUANTITY='LAYER HEIGHT', ID='whatever' /
```

produces a time history of the smoke layer height at $x = 2$ and $y = 3$ between $z = 0$ and $z = 3$. If multiple meshes are being used, the vertical path *cannot* cross mesh boundaries.

14.3.4 The True Gas Temperature vs. the Measured Gas Temperature

The output quantity THERMOCOUPLE is the temperature of the thermocouple itself, usually close to the gas temperature, but not always. It is determined by solving the following equation for T_{TC} iteratively [17]

$$\varepsilon_{TC}(\sigma T_{TC}^4 - U/4) + h(T_{TC} - T_g) = 0 \tag{14.13}$$

where ε_{TC} is the emissivity of the thermocouple, U is the integrated radiative intensity, T_g is the true gas temperature, and h is the heat transfer coefficient to a small sphere, $h = k_a \mathrm{Nu}/\mathrm{Pr}/d_{TC}$. The bead BEAD_DIAMETER and BEAD_EMISSIVITY are given on the associated PROP line. See the discussion on heat transfer to a water droplet in the Technical Reference Guide for details of the convective heat transfer to a small sphere.

14.3.5 Heat Fluxes and Thermal Radiation

There are various ways of recording the heat flux at a solid boundary. If you want to record the *net* heat flux to the surface, $\dot{q}_c'' + \dot{q}_r''$, use the QUANTITY called 'NET HEAT FLUX'. The individual components, the *net* convective and radiative fluxes, are 'CONVECTIVE HEAT FLUX' and 'RADIATIVE HEAT FLUX', respectively. If you want to compare predicted heat flux with a measurement, you often need to use 'GAUGE

---

[2]Note that in FDS 5 and beyond, these quantities are no longer available as slice files.

HEAT FLUX'. The difference between 'NET HEAT FLUX' and 'GAUGE HEAT FLUX' is that the former is the rate at which energy is absorbed by the solid surface; the latter is the amount of energy that would be absorbed if the surface were cold (or some specified temperature):

$$\dot{q}_r''/\varepsilon + \dot{q}_c'' + h(T_w - T_\infty) + \sigma(T_w^4 - T_\infty^4)$$

If the heat flux gauge used in an experiment has a temperature other than ambient, set GAUGE_TEMPERATURE on the PROP line associated with the device. When comparing against a radiometer measurement, use RADIOMETER:

$$\dot{q}_r''/\varepsilon + \sigma(T_w^4 - T_\infty^4)$$

For diagnostic purposes it is sometimes convenient to output the 'INCIDENT HEAT FLUX':

$$\dot{q}_r''/\varepsilon + \sigma T_w^4 + \dot{q}_c''$$

All of the above heat flux output quantities are defined at a solid surface. However, 'RADIATIVE HEAT FLUX GAS' acts like a radiometer that is not attached to a solid surface. This quantity integrates the incoming radiative flux over 2π solid angles around the vector defined by ORIENTATION, a triplet of real numbers that defines the orientation of the device. For example,
ORIENTATION=-1.0,0.0,0.0
means that the device points in the negative x direction. Unlike IOR, the ORIENTATION can be in any direction, not just those associated with the three coordinate directions.

Note that the sign of the output of heat flux is different than the sign of the input of a heat flux. A positive output quantity for heat flux means heat is being transferred into the surface.

14.3.6 Droplet Output Quantities

Droplet Quantities on Solid Surfaces

It is possible to record various properties of droplets and particles. Some of the output quantities are associated with solid boundaries. For example, 'MPUA' is the Mass Per Unit Area of the droplets named PART_ID. Likewise, 'AMPUA' is the Accumulated Mass Per Unit Area. Both of these are given in units of kg/m^2. Think of these outputs as measures of the instantaneous mass density per unit area, and the accumulated total, respectively. The accumulated total is analogous to a "bucket test," where the droplets are collected in buckets and the total mass determined at the end of a given time period. The cooling of a solid surface by droplets of a given type is given by 'CPUA', the Cooling Per Unit Area in units of kW/m^2.

Be aware of the fact that the default behavior for droplets hitting the "floor," that is, the plane $z =$ ZMIN, is to disappear (POROUS_FLOOR=.TRUE. on the MISC line). In this case, 'MPUA' will be zero, but 'AMPUA' will not. FDS stores the droplet mass just before removing the droplet from the simulation for the purpose of saving CPU time.

In the test case **bucket_test**, a single sprinkler is mounted 10 cm below a 5 m ceiling. Water flows for 30 s at a constant rate of 180 L/min (ramped up and down in 1 s). The simulation continues for another 10 s to allow water drops time to reach the floor. The total mass of water discharged is

$$180 \, \frac{\text{L}}{\text{min}} \times 1 \, \frac{\text{kg}}{\text{L}} \times \frac{1}{60} \, \frac{\text{min}}{\text{s}} \times 30 \, \text{s} = 90 \, \text{kg} \tag{14.14}$$

In the simulation, the boundary quantity water_drops_AMPUA (Accumulated Mass Per Unit Area) records the total water mass per unit area (kg/m^2), analogous to actual buckets the size of a grid cell. Summing the values of water_drops_AMPUA over the entire floor yields 88.3 kg. Where is the missing water? Some

droplets evaporate, and some droplets fly beyond the computational domain. Note that there are no actual "buckets" in the simulation.

The accumulated water mass at the floor is extracted from the boundary (BNDF) file via the command line program **fds2ascii**. Here is a transcript of the session used to convert the binary FDS output file into ASCII format:

```
>> fds2ascii
  Enter Job ID string (CHID):
bucket_test
  What type of file to parse?
  PL3D file? Enter 1
  SLCF file? Enter 2
  BNDF file? Enter 3
3
  Enter Sampling Factor for Data?
  (1 for all data, 2 for every other point, etc.)
1
  Limit the domain size? (y or n)
y
  Enter min/max x, y and z
-5 5 -5 5 0 1
  1   MESH   1, water_drops_AMPUA
  Enter starting and ending time for averaging (s)
35 36
  Enter orientation: (plus or minus 1, 2 or 3)
3
  Enter number of variables
1
 Enter boundary file index for variable 1
1
 Enter output file name:
bucket_test_fds2ascii.csv
  Writing to file...      bucket_test_fds2ascii.csv
```

Note that there really is no need to time-average the results. The quantity is inherently accumulating. Also, the "orientation" refers to direction of the surface. In this case, we're interested in the positive *z* direction, or 3.

Droplet Mass and Fluxes in Gas Phase

Away from solid surfaces, 'MPUV' is the Mass Per Unit Volume of the droplets as they fly through the air, in units of kg/m^3. 'DROPLET FLUX X', 'DROPLET FLUX Y', and 'DROPLET FLUX Z' produce *only* slice and Plot3D files of the mass flux of droplets in the *x*, *y*, and *z* directions, respectively, in units of kg/m^2/s.

Local Spray Properties

Detailed experimental measurements of sprays are often performed using Phase Doppler Particle Analysis (PDPA) which can be used to obtain information on the droplet size distribution, speed and concentration. Special device type has been defined to simulate the PDPA measurement. The actual quantity to measure, and the details of the measurement are defined using an associated PROPerty. Note that in FDS, the PDPA device cannot produce complete droplet size distributions, but only various mean properties.

The PDPA device output at time *t* is computed as

$$f(t) = \frac{1}{\min(t, t_e) - t_s} \int_{t_s}^{\min(t, t_e)} \left(\frac{\sum_i n_i d_i^m}{\sum_i n_i d_i^n} \right)^{1/(m-n)} x dt \qquad (14.15)$$

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where x is the quantity to be measured. The summation goes over all the particles within a sphere with radius `PDPA_RADIUS` and centered at the location given by the device `XYZ`. The properties of the PDPA device are defined using the following keywords on the `PROP` line:

`PART_ID` Name of the particle group to limit the computation to. Use `'ALL'` to account for all particles.

`PDPA_START` t_s, starting time of time integration in seconds. PDPA output is always a running average over time. As the spray simulation may contain some initial transient phase, it may be useful to specify the starting time of data collection.

`PDPA_END` t_e, ending time of time integration in seconds.

`PDPA_M` m, exponent of diameter.

`PDPA_N` n, exponent of diameter. In case $m = n$, the exponent $1/(m-n)$ is removed from the formula.

`PDPA_RADIUS` Radius (m) of the sphere, centered at the device location, inside which the particles are monitored.

`QUANTITY` Particle property that is used for variable x. Possible variables are `'VELOCITY'`, `'U-VELOCITY'`, `'V-VELOCITY'`, `'W-VELOCITY'`, `'TEMPERATURE'` and `'NUMBER CONCENTRATION'`. Leave unspecified to compute mean diameters.

The following example is used to measure the Sauter mean diameter D_{32} of the particle type `'water drops'`, starting from time 5.0 s.

```
&PROP ID='pdpa_d32'
      PART_ID='water drops'
      PDPA_M=3
      PDPA_N=2
      PDPA_RADIUS=0.01
      PDPA_START=5.0 /
&DEVC XYZ=0.0,0.0,1.0, QUANTITY='PDPA', PROP_ID='pdpa_d32' /
```

14.3.7 Interfacing with Structural Models

FDS solves a one-dimensional heat conduction equation for each boundary cell marking the interface between gas and solid, assuming that material properties for the material layer(s) are provided. The results can be transferred (via either `DEVC` or `BNDF` output) to other models that predict the mechanical response of the walls or structure. For many applications, the 1-D solution of the heat conduction equation is adequate, but in situations where it is not, another approach can be followed. FDS includes a calculation of the Adiabatic Surface Temperature (AST), a quantity that is representative of the heat flux to a solid surface. Following the idea proposed by Ulf Wickstrom [18], the following equation can be solved via a simple iterative technique to determine an effective gas temperature, T_{AST}:

$$\dot{q}_r'' + \dot{q}_c'' = \varepsilon\sigma\left(T_{\mathrm{AST}}^4 - T_w^4\right) + h(T_{\mathrm{AST}} - T_w) \tag{14.16}$$

The sum $\dot{q}_r'' + \dot{q}_c''$ is the *net* heat flux onto the solid surface, whose temperature is T_w. The heat fluxes and surface temperature are computed in FDS, and they are inter-dependent. The computed wall temperature affects the net heat flux and vice versa. However, because FDS only computes the solution to the 1-D heat conduction equation in the solid, it may be prone to error if lateral heat conduction within the solid is

significant. Thus, in some scenarios neither the FDS-predicted heat fluxes or the surface temperature can be used as an accurate indicator of the thermal insult from the hot, smokey gases onto solid objects.

Of course, both the heat fluxes, $\dot{q}''_r$ and $\dot{q}''_c$, and the surface temperature, T_w can be passed from FDS to the other model, and suitable corrections can be made based on a presumably more accurate prediction of the solid temperature. Alternatively, the single quantity, T_{AST}, can be transferred, as this is the temperature that the solid surface effectively "sees." It represents the gas phase thermal environment, however complicated, but it does not carry along the uncertainty associated with the simple solid phase heat conduction model within FDS. Obviously, the objective in passing information to a more detailed model is to get a better prediction of the solid temperature (and ultimately its mechanical response) than FDS can provide.

14.3.8   Useful Solid Phase Outputs

In addition to the `PROF`ile output, there are various additional quantities that are useful for monitoring reacting surfaces. For example, `'WALL THICKNESS'` gives the overall thickness of the solid surface element. `'SURFACE DENSITY'` gives the overall mass per unit area for the solid surface element, computed as an integral of material density over wall thickness. Both quantities are available both as `DEVC` and `BNDF`.

To record the change in a material component's density with time, use the output quantity `'SOLID DENSITY'` in the following way:

```
&DEVC ID='...', XYZ=..., IOR=3, QUANTITY='SOLID DENSITY', MATL_ID='wood', DEPTH=0.001 /
```

This produces a time history of the density of the material referred to as `'wood'` on a `MATL` line. The density is recorded 1 mm beneath the surface which is oriented in the positive z direction. Note that if `'wood'` is part of a mixture, the density represents the mass of `'wood'` per unit volume of the mixture. Note also that `'SOLID DENSITY'` is only available as a `DEVC` (device) quantity.

14.3.9   Fractional Effective Dose (FED)

The Fractional Effective Dose index (FED), developed by Purser [19], is a commonly used measure of human incapasitation due to the combustion gases. The present version of FDS uses only the concentrations of the gases CO, CO_2, and O_2 to calculate the FED value as

$$\text{FED}_{\text{tot}} = \text{FED}_{\text{CO}} \times \text{HV}_{\text{CO}_2} + \text{FED}_{\text{O}_2} \tag{14.17}$$

The fraction of an incapacitating dose of CO is calculated as

$$\text{FED}_{\text{CO}} = 4.607 \times 10^{-7} \left(C_{\text{CO}} \right)^{1.036} t \tag{14.18}$$

where t is time in seconds and C_{CO} is the CO concentration (ppm). The fraction of an incapacitating dose of low O_2 hypoxia is calculated as

$$\text{FED}_{\text{O}_2} = \frac{t}{60 \exp\left[8.13 - 0.54 \left(20.9 - C_{\text{O}_2} \right) \right]} \tag{14.19}$$

where C_{O_2} is the O_2 concentration (volume per cent). The hyperventilation factor induced by carbon dioxide is calculated as

$$\text{HV}_{\text{CO}_2} = \frac{\exp(0.1930 C_{\text{CO}_2} + 2.0004)}{7.1} \tag{14.20}$$

where C_{CO_2} is the CO_2 concentration (percent).

Note that the spatial integration features (Section 14.3.10) cannot be used with FED output because FED makes use of the `TIME INTEGRAL` (Section 14.3.11). For the same reason, FED output is only available as a point measurement.

14.3.10 Spatially-Integrated Outputs

A useful feature of a device (`DEVC`) is to specify an output quantity along with a desired statistic. For example,

```
&DEVC XB=2.3,4.5,2.8,6.7,3.6,7.8, QUANTITY='TEMPERATURE', ID='maxT', STATISTICS='MAX' /
```

causes FDS to write out the maximum gas phase temperature over the volume bounded by `XB`. Note that it does not compute the maximum over the entire computational domain, just the specified volume, and this volume must lie within a single mesh. Other `STATISTICS` are discussed below. Note that some are appropriate for gas phase output quantities, some for solid phase, and some for both.

For solid phase output quantities, like heat fluxes and surface temperatures, the specification of a `SURF_ID` along with the appropriate statistic limits the calculation to only those surfaces. You can further limit the search by using the sextuplet of coordinates `XB` to force FDS to only compute statistics for surface cells within the given volume. Be careful to account for the fact that the solid surface might shift to conform to the underlying numerical grid. Also, be careful not to specify a volume that extends beyond a single mesh. Note that you do not (and should not) specify an orientation via the parameter `IOR` when using a spatial statistic. `IOR` is only needed to find a specific point on the solid surface.

> Use the `STATISTICS` feature with caution because it demands that FDS evaluate the given `QUANTITY` in all gas or solid phase cells.

Minimum or Maximum Value

For a given gas phase scalar output quantity defined at the center of each grid cell, ϕ_{ijk}, `STATISTICS='MIN'` or `STATISTICS='MAX'` computes the minimum or maximum value, respectively

$$\min_{ijk} \phi_{ijk} \quad ; \quad \max_{ijk} \phi_{ijk} \tag{14.21}$$

over the cells that are included in the specified volume bounded by `XB`. Note that this statistic is only appropriate for gas phase quantities. Note also that you must specify a volume to sum over via the coordinate parameters, `XB`, all of which must be contained within the same mesh.

Average Value

For a given gas phase scalar output quantity defined at the center of each grid cell, ϕ_{ijk}, `STATISTICS='MEAN'` computes the average value,

$$\frac{1}{N} \sum_{ijk} \phi_{ijk} \tag{14.22}$$

over the cells that are included in the specified volume bounded by `XB`. Note that this statistic is only appropriate for gas phase quantities. Note also that you must specify a volume to sum over via the coordinate parameters, `XB`, all of which must be contained within the same mesh.

Volume-Weighted Mean

For a given gas phase output quantity, $\phi(x,y,z)$, `STATISTICS='VOLUME MEAN'` produces the discrete analog of

$$\frac{1}{V} \int \phi(x,y,z) \, dx \, dy \, dz \tag{14.23}$$

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which is very similar to 'MEAN', but it weights the values according to the relative size of the mesh cell. Note that this statistic is only appropriate for gas phase quantities. Note also that you must specify a volume to sum over via the coordinate parameters, XB, all of which must be contained within the same mesh.

Mass-Weighted Mean

For a given gas phase output quantity, $\phi(x,y,z)$, STATISTICS='MASS MEAN' produces the discrete analog of

$$\frac{\int \rho(x,y,z)\,\phi(x,y,z)\,dx\,dy\,dz}{\int \rho\,dx\,dy\,dz} \tag{14.24}$$

which is similar to 'VOLUME MEAN', but it weights the values according to the relative mass of the mesh cell. Note that this statistic is only appropriate for gas phase quantities. Note also that you must specify a volume to sum over via the coordinate parameters, XB, all of which must be contained within the same mesh.

Volume Integral

For a given gas phase output quantity, $\phi(x,y,z)$, STATISTICS='VOLUME INTEGRAL' produces the discrete analog of

$$\int \phi(x,y,z)\,dx\,dy\,dz \tag{14.25}$$

Note that this statistic is only appropriate for gas phase quantities, in particular those whose units involve m^{-3}. For example, heat release rate per unit volume is an appropriate output quantity. Note also that you must specify a volume to sum over via the coordinate parameters, XB, all of which must be contained within the same mesh.

Mass Integral

For a given gas phase output quantity, $\phi(x,y,z)$, STATISTICS='MASS INTEGRAL' produces the discrete analog of

$$\int \rho(x,y,z)\,\phi(x,y,z)\,dx\,dy\,dz \tag{14.26}$$

Note that this statistic is only appropriate for gas phase quantities. Note also that you must specify a volume to sum over via the coordinate parameters, XB, all of which must be contained within the same mesh.

Area Integral

For a given gas phase output quantity, $\phi(x,y,z)$, STATISTICS='AREA INTEGRAL' produces the discrete analog of

$$\int \phi(x,y,z)\,dA \tag{14.27}$$

where dA depends on the coordinates you specify for XB. Note that this statistic is only appropriate for gas phase quantities, in particular those whose units involve m^{-2}. For example, the quantity 'MASS FLUX X' along with SPEC_ID='my gas' is an appropriate output quantity if you want to know the mass flux of the gas species that you have named 'my gas' through an area normal to the x direction. Note also that you must specify an area to sum over via the coordinate parameters, XB, all of which must be contained within the same mesh.

Surface Integral

For a given solid phase output quantity, ϕ, `STATISTICS='SURFACE INTEGRAL'` produces the discrete analog of

$$\int \phi \, dA \tag{14.28}$$

Note that this statistic is only appropriate for solid phase quantities, in particular those whose units involve m^{-2}. For example, the various heat and mass fluxes are appropriate output quantities.

Mass and Energy Flows

The net flow of mass and energy into or out of compartments can be useful for many applications. There are several outputs that address these. All are prescribed via the device (`DEVC`) namelist group only. For example:

```
&DEVC XB=0.3,0.5,2.1,2.5,3.0,3.0, QUANTITY='MASS FLOW', ID='whatever' /
```

outputs the net integrated mass flux through the given planar area, oriented in the positive z direction, in this case. The three flows – `'VOLUME FLOW'`, `'MASS FLOW'`, and `'HEAT FLOW'` are defined:

$$\dot{V} = \int \mathbf{u} \cdot d\mathbf{S}$$

$$\dot{m} = \int \rho \mathbf{u} \cdot d\mathbf{S}$$

$$\dot{q} = \int c_p \rho (T - T_\infty) \mathbf{u} \cdot d\mathbf{S}$$

The addition of a + or − to the `QUANTITY` names yields the integral of the flow in the positive or negative direction only. In other words, if you want to know the mass flow out of a compartment, use `'MASS FLOW +'` or `'MASS FLOW −'`, depending on the orientation of the door.

14.3.11 Temporally-Integrated Outputs

In addition to the spatial statistics, a time integral of an `DEVC` output can be computed by specifying `STATISTICS = 'TIME INTEGRAL'` on the `DEVC` line. This produces a discrete analog of

$$\int_{t_0}^{t} \phi(\tau) \, d\tau \tag{14.29}$$

Note that the spatial and time integrals can not be used simultaneously.

14.3.12 Wind and the Pressure Coefficient

In the field of wind engineering, a commonly used quantity is known as the `PRESSURE_COEFFICIENT`:

$$C_p = \frac{p - p_\infty}{\frac{1}{2}\rho_\infty U^2} \tag{14.30}$$

p_∞ is the ambient, or "free stream" pressure, and ρ_∞ is the ambient density. The parameter U is the free-stream wind speed, given as `CHARACTERISTIC_VELOCITY` on the `PROP` line

```
&BNDF QUANTITY='PRESSURE COEFFICIENT', PROP_ID='whatever' /
&DEVC ID='pressure tap', XYZ=..., IOR=2, QUANTITY='PRESSURE COEFFICIENT', PROP_ID='whatever' /
&PROP ID='whatever', CHARACTERISTIC_VELOCITY=3.4 /
```

Thus, you can either paint values of C_p at all surface points, or create a single time history of C_p using a single device at a single point.

14.3.13 Dry Volume and Mass Fractions

During actual experiments, species such as CO and CO_2 are typically measured "dry"; that is, the water vapor is removed from the gas sample prior to analysis. For easier comparison of FDS predictions with measured data, you can specify the logical parameter DRY on a DEVC line that reports the 'MASS FRACTION' or 'VOLUME FRACTION' of a species when using the mixture fraction combustion model. For example, the first line reports the actual volume fraction of CO, and the second line reports the output of a gas analyzer in a typical experiment.

```
&DEVC ID='wet CO', XYZ=..., QUANTITY='VOLUME FRACTION', SPEC_ID='carbon monoxide' /
&DEVC ID='dry CO', XYZ=..., QUANTITY='VOLUME FRACTION', SPEC_ID='carbon monoxide', DRY=.TRUE. /
```

14.4 Extracting Numbers from the Output Data Files

Often it is desired to present results of calculations in some form other than those offered by Smokeview. In this case, there is a short Fortran 90 program called **fds2ascii.f90**, with a PC compiled version called **fds2ascii.exe**. To run the program, just type

```
fds2ascii
```

at the command prompt. You will be asked a series of questions about which type of output file to process, what time interval to time average the data, and so forth. A single file is produced with the name **CHID_fds2ascii.csv**. A typical command line session looks like this:

```
>> fds2ascii
  Enter Job ID string (CHID):
bucket_test
  What type of file to parse?
  PL3D file? Enter 1
  SLCF file? Enter 2
  BNDF file? Enter 3
3
  Enter Sampling Factor for Data?
  (1 for all data, 2 for every other point, etc.)
1
  Limit the domain size? (y or n)
y
  Enter min/max x, y and z
-5 5 -5 5 0 1
  1   MESH  1, WALL TEMPERATURE
  Enter starting and ending time for averaging (s)
35 36
  Enter orientation: (plus or minus 1, 2 or 3)
3
  Enter number of variables
1
 Enter boundary file index for variable 1
1
 Enter output file name:
bucket_test_fds2ascii.csv
  Writing to file...      bucket_test_fds2ascii.csv
```

These commands tell **fds2ascii** that you want to convert (binary) boundary file data into a text file. You want to sample every data point within the specified volume, you want only those surfaces that point upwards (+3 orientation), you only want 1 variable (only one is listed anyway and its index is 1 – that is just the number

used to list the available files). The data will be time-averaged, and it will be output to a file listed at the end of the session.

14.5 Summary of Frequently-Used Output Quantities

Table 14.1, spread over the following pages, summarizes the various Output Quantities. The column "File Type" lists the allowed output files for the quantities. "B" is for Boundary (`BNDF`), "D" is for Device (`DEVC`), "I" is for Iso-surface (`ISOF`), "P" is for Plot3D, "PA" for PArticle (`PART`), "S" is for Slice (`SLCF`). Be careful when specifying complicated quantities for Iso-surface or Plot3D files, as it requires computation in every gas phase cell.

For those output quantities that require a species name via `SPEC_ID`, the species implicitly defined when doing a mixture fraction calculation are as follows:

```
fuel
oxygen
nitrogen
water vapor
carbon dioxide
carbon monoxide
hydrogen
soot
other
```

As an example of how to use the species names, suppose you want to calculate the integrated mass flux of carbon monoxide through a horizontal plane, like the total amount entrained in a fire plume. Use a "device" as follows

```
&DEVC ID='CO_flow', XB=-5,5,-5,5,2,2, QUANTITY='MASS FLUX Z', SPEC_ID='carbon monoxide',
      STATISTICS='AREA INTEGRAL' /
```

Here, the `ID` is just a label in the output file. The use of lower case letters for the `SPEC_ID` indicates that you want to record the mass flow of the CO that is implicitly defined by the mixture fraction variables. This is the default combustion model in FDS. If you have defined a species explicitly via a `SPEC` line, you can specify that instead.

The format of certain output quantities changed, starting with FDS version 5.2, but the older names originating with version 5.0 will still be accepted. The new convention is that when an output quantity is related to a particular gas species or particle type, then you must specify the appropriate `SPEC_ID` or `PART_ID` on the same input line. Also note that the use of underscores in output quantity names has been eliminated – just remember that all output quantity names ought to be in single quotes.

Table 14.1: Summary of frequently used output quantities.

QUANTITY	Symbol	Units	File Type
ABSORPTION COEFFICIENT	κ (Section 11.3)	1/m	D,I,P,S
ACTUATED SPRINKLERS	Number of actuated sprinklers		D
ADIABATIC SURFACE TEMPERATURE	See Section 14.3.7	°C	B,D
AMPUA**	See Section 14.3.6	kg/m^2	B,D
ASPIRATION	See Section 13.3.6	%	D
AVERAGE SPECIFIC HEAT	$\bar{c}_p$	kJ/kg/K	D,I,P,S
BACK WALL TEMPERATURE	See Section 14.2.2	°C	B,D
BURNING RATE	$\dot{m}''_f$	kg/m^2/s	B,D
CHAMBER OBSCURATION	See Section 13.3.4	%/m	D
CONDUCTIVITY	k	W/m/k	D,I,P,S
CONTROL	See Section 13.5		D
CONVECTIVE HEAT FLUX	$\dot{q}''_c$ (Section 14.3.5)	kW/m^2	B,D
CPUA**	See Section 14.3.6	kW/m^2	B,D
CPU TIME	Elapsed CPU time	s	D
DENSITY	ρ or ρY_α with SPEC_ID	kg/m^3	D,I,P,S
DIVERGENCE	$\nabla \cdot \mathbf{u}$	s^{-1}	D,I,P,S
DROPLET FLUX X**	See Section 14.3.6	kg/m^2/s	P,S
DROPLET FLUX Y**	See Section 14.3.6	kg/m^2/s	P,S
DROPLET FLUX Z**	See Section 14.3.6	kg/m^2/s	P,S
DROPLET DIAMETER	$2r_d$	μm	PA
DROPLET VELOCITY	$|\mathbf{u}_d|$	m/s	PA
DROPLET TEMPERATURE	T_d	°C	PA
DROPLET MASS	m_d	kg	PA
DROPLET AGE	t_d	s	PA
ENTHALPY	$\sum \rho Y_\alpha \int_0^T c_{p,\alpha}(T')\,dT'$	kJ/m^3	D,I,P,S
FED	See Section 14.3.9		D
GAUGE HEAT FLUX	See Section 14.3.5	kW/m^2	B,D
H	$H = |\mathbf{u}|^2/2 + \tilde{p}/\rho_0$	(m/s)^2	D,I,P,S
HEAT FLOW	See Section 14.3.10	kW	D
NET HEAT FLUX	See Section 14.3.5	kW/m^2	B,D
HRR	$\int \dot{q}'''\,dV$	kW	D
HRRPUV	$\dot{q}'''$	kW/m^3	D,I,P,S
INCIDENT HEAT FLUX	See Section 14.3.5	kW/m^2	B,D
INSIDE WALL TEMPERATURE	See Section 14.2.2	°C	D
ITERATION	Number of time steps		D
LAYER HEIGHT	See Section 14.3.3	m	D
LINK TEMPERATURE	See Section 13.3.3	°C	D
LOWER TEMPERATURE	See Section 14.3.3	°C	D
MASS FLOW	See Section 14.3.10	kg/s	D
MASS FLUX*	Mass flux at solid surface	kg/m^2/s	B,D
MASS FLUX X*	$\rho u Y_\alpha$	kg/m^2/s	D,I,P,S
MASS FLUX Y*	$\rho v Y_\alpha$	kg/m^2/s	D,I,P,S
MASS FLUX Z*	$\rho w Y_\alpha$	kg/m^2/s	D,I,P,S

Table 14.1: Summary of frequently used output quantities (continued).

QUANTITY	Symbol	Units	File Type
MASS FRACTION[*]	Y_α	kg/kg	D,I,P,S
MIXTURE FRACTION	Z	kg/kg	D,I,P,S
MPUA[**]	See Section 14.3.6	kg/m^2	B,D
MPUV[**]	See Section 14.3.6	kg/m^3	D,P,S
NORMAL VELOCITY	Wall normal velocity	m/s	D,B
OPTICAL DENSITY	$K/2.3$ (Section 14.3.2)	1/m	D,I,P,S
EXTINCTION COEFFICIENT	K (Section 14.3.2)	1/m	D,I,P,S
PATH OBSCURATION	See Section 13.3.5	%	D
PRESSURE	Perturbation pressure, $\tilde{p}$	Pa	D,I,P,S
PRESSURE COEFFICIENT	C_p (Section 14.3.12)		B,D
PRESSURE ZONE	See Section 9.6		D,S
RADIATIVE HEAT FLUX	See Section 14.3.5	kW/m^2	B,D
RADIATIVE HEAT FLUX GAS	See Section 14.3.5	kW/m^2	D
RADIOMETER	See Section 14.3.5	kW/m^2	B,D
RELATIVE HUMIDITY	Relative humidity	%	D,I,P,S
SOOT VOLUME FRACTION	$\rho Y_s(Z)/\rho_s$	mol/mol	D,I,P,S
SPECIFIC ENTHALPY	$\sum Y_\alpha \int_0^T c_{p,\alpha}(T')\,dT'$	kJ/kg	D,I,P,S
SPECIFIC HEAT	c_p	kJ/kg/K	D,I,P,S
SPRINKLER LINK TEMPERATURE	See Section 13.3.1	°C	D
SOLID DENSITY	See Section 14.3.8	kg/m^3	D
SURFACE DENSITY	See Section 14.3.8	kg/m^2	B,D
TEMPERATURE	T (Section 14.3.4)	°C	D,I,P,S
THERMOCOUPLE	T_{TC} (Section 14.3.4)	°C	D
TIME	t (Section 13.1)	s	D
TIME STEP	δt, Numerical time step	s	D
U-VELOCITY	u	m/s	D,I,P,S
V-VELOCITY	v	m/s	D,I,P,S
W-VELOCITY	w	m/s	D,I,P,S
UPPER TEMPERATURE	See Section 14.3.3	°C	D
VELOCITY	$\sqrt{u^2 + v^2 + w^2}$	m/s	D,I,P,S
VISCOSITY	μ	kg/m/s	D,I,P,S
VISIBILITY	$S = C/K$ (Section 14.3.2)	m	D,I,P,S
VOLUME FLOW	See Section 14.3.10	m^3/s	D
VOLUME FRACTION[*]	X_α	mol/mol	D,I,P,S
WALL CLOCK TIME	Elapsed wall clock time	s	D
WALL TEMPERATURE	T_w	°C	B,D
WALL THICKNESS	See Section 14.3.8	m	B,D

[*]   Quantity requires the specification of a gas species using SPEC_ID.
[**]   Quantity requires the specification of a particle name using PART_ID.

14.6 Summary of Infrequently-Used Output Quantities

Table 14.2 below lists some less often used output quantities. These are mainly used for diagnostic purposes. Explanations for most can be found in Volume 1 of the FDS Technical Reference Guide [1].

Table 14.2: Summary of *infrequently* used output quantities.

QUANTITY	Symbol	Units	File Type
ADD	Average Droplet Density	kg/m^3	D,I,P,S
ADT	Average Droplet Temperature	°C	D,I,P,S
DROPLET PHASE	Orientation of droplet		PA
EMISSIVITY	Surface emissivity (usually constant)		B,D
F_X, F_Y, F_Z	Momentum terms, F_x, F_y, F_z	m/s^2	D,I,P,S
GAS TEMPERATURE	Gas Temperature near wall	°C	B,D
HEAT TRANSFER COEFFICIENT	Convective heat transfer	kW/m^2/K	B,D
HP	$\mathcal{H}'$ (pressure correction)	(m/s)^2	D,I,P,S
HRRPUL	$\int \dot{q}''' \, dx \, dy$	kW/m	D
INTEGRATED INTENSITY	$U = \int I d\mathbf{s}$	kW/m^2	D,I,P,S
KINETIC ENERGY	$(u^2 + v^2 + w^2)/2$	(m/s)^2	D,I,P,S
MIXING TIME	Combustion mixing time	s	D,I,P,S
PDPA	Droplet diagnostics		D
RADIATION LOSS	$\nabla \cdot \mathbf{q}_r''$	kW/m^3	D,I,P,S
STRAIN RATE X	$\partial w/\partial y + \partial v/\partial z$	1/s	D,I,P,S
STRAIN RATE Y	$\partial u/\partial z + \partial w/\partial x$	1/s	D,I,P,S
STRAIN RATE Z	$\partial v/\partial x + \partial u/\partial y$	1/s	D,I,P,S
VORTICITY X	$\partial w/\partial y - \partial v/\partial z$	1/s	D,I,P,S
VORTICITY Y	$\partial u/\partial z - \partial w/\partial x$	1/s	D,I,P,S
VORTICITY Z	$\partial v/\partial x - \partial u/\partial y$	1/s	D,I,P,S
WATER RADIATION LOSS	$\nabla \cdot \mathbf{q}_r''$ due to water droplets	kW/m^3	D,I,P,S

Chapter 15

Alphabetical List of Input Parameters

This Appendix lists all of the input parameters for FDS in separate tables grouped by Namelist, these tables are in alphabetical order along with the parameters within them. This is intended to be used as a quick reference and does not replace reading the detailed description of the parameters in the main body of this guide. See Table 5.1 for a cross-reference of relevant sections and the tables in this Appendix. The reason for this statement is that many of the listed parameters are mutually exclusive – specifying more than one can cause the program to either fail or run in an unpredictable manner. Also, some of the parameters trigger the code to work in a certain mode when specified. For example, specifying the thermal conductivity of a solid surface triggers the code to assume the material to be thermally-thick, mandating that other properties be specified as well. Simply prescribing as many properties as possible from a handbook is bad practice. Only prescribe those parameters which are necessary to describe the desired scenario.

15.1 `BNDF` (Boundary File Parameters)

Table 15.1: For more information see Section 14.2.4.

BNDF (Boundary File Parameters)				
`CELL_CENTERED`	Logical	Do not do corner averaging		.FALSE.
`FYI`	Character	Comment String (has no effect)		
`PART_ID`	Character	Particle identifier (if needed)		
`PROP_ID`	Character	Property identifier (if needed)		
`RECOUNT_DRIP`	Logical	Adds mass to AWMPUA for each drop impact	.FALSE.	
`QUANTITY`	Character	Quantity to visualize		
`SPEC_ID`	Character	Species identifier (if needed)		

15.2 `CLIP` (MIN/MAX Clipping Parameters)

Table 15.2: For more information see Section 6.6.

CLIP (Specified Upper and Lower Limits)				
`FYI`	Character	Comment String (has no effect)		
`MAXIMUM_DENSITY`	Real	Maximum Gas Density	kg/m^3	
`MAXIMUM_MASS_FRACTION`	Real Array	Maximum Gas Mass Fraction	kg/kg	
`MAXIMUM_TEMPERATURE`	Real	Maximum Gas Temperature	°C	
`MINIMUM_DENSITY`	Real	Minimum Gas Density	kg/m^3	
`MINIMUM_MASS_FRACTION`	Real Array	Minimum Gas Mass Fraction	kg/kg	
`MINIMUM_TEMPERATURE`	Real	Maximum Gas Temperature	°C	

15.3 `CTRL` (Control Function Parameters)

Table 15.3: For more information see Section 13.5.

CTRL (Control Function Parameters)				
`DELAY`	Real	Time delay	s	0.
`FUNCTION_TYPE`	Character	Type of control function		
`ID`	Character	IDentifier		
`INITIAL_STATE`	Logical	Initial state of control function		.FALSE.
`INPUT_ID`	Char. Array	DEVC and/or CTRL input IDs		
`LATCH`	Logical	Control function changes state only once		.TRUE.
`N`	Integer	Number of .TRUE. INPUTs		1
`ON_BOUND`	Character	Active edge of a DEADBAND		LOWER
`RAMP_ID`	Character	ID for a CUSTOM ramp controller		
`SETPOINT(2)`	Real	Lower and upper bound of a DEADBAND		

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15.4 `DEVC` (Device Parameters)

Table 15.4: For more information see Section 13.1.

DEVC (Device Parameters)				
BYPASS_FLOWRATE	Real	Aspiration smoke detector parameter	kg/s	0
CTRL_ID	Character	Associated CTRL line		
DELAY	Real	Transport time for an aspiration detector	s	0
DEVC_ID	Character	Associated DEVC line for aspiration detector		
DEPTH	Real	Depth into surface for internal wall temp	m	0
FLOWRATE	Real	Suction flowrate for an aspiration detector	kg/s	0
FYI	Character	Comment String (has no effect)		
IOR	Integer	Index of Orientation ($\pm 1, \pm 2, \pm 3$)		
ID	Character	Identifying label for output		
INITIAL_STATE	Logical	Initial state of device		.FALSE.
LATCH	Logical	Device cannot change state multiple times		.TRUE.
MATL_ID	Character	Material identifier (if needed)		
ORIENTATION	Real Triplet	Direction vector		0,0,-1
PART_ID	Character	Particle identifier (if needed)		
PROP_ID	Character	Associated PROPerty line		
QUANTITY	Character	Name of Quantity to output		
ROTATION	Real Triplet	Rotation Angle	deg	0
SETPOINT	Real	Value at which device changes state		
SPEC_ID	Character	Species identifier (if needed)		
STATISTICS	Character	See Section 14.3.10		
SURF_ID	Character	See Section 14.3.10		
TIME_AVERAGED	Logical	See Section 13.2		.TRUE.
TRIP_DIRECTION	Integer	Sign of derivative at first state change		1
XB(6)	Real Sextuplet	Coordinates of non-point measurement	m	
XYZ	Real Triplet	Physical coordinates	m	

15.5 `DUMP` (Output Parameters)

Table 15.5: For more information see Section 14.1.

DUMP (Output Parameters)				
CHECK_VOLUME_FLOW	Logical	See Section 6.4.4		.FALSE.
COLUMN_DUMP_LIMIT	Logical	Limit text output to 255 columns		.TRUE.
CTRL_COLUMN_LIMIT	Integer	Number of columns in CTRL file		254
DEVC_COLUMN_LIMIT	Integer	Number of columns in DEVC file		254
DT_BNDF	Real	Boundary dump interval	s	$2\Delta t$ /NFRAMES
DT_CTRL	Real	Control status dump interval	s	Δt /NFRAMES
DT_DEVC	Real	Device output dump interval	s	Δt /NFRAMES
DT_FLUSH	Real	See Section 14.1	s	Δt /NFRAMES

DUMP (Output Parameters)					
DT_HRR	Real	Heat release dump interval		s	Δt/NFRAMES
DT_ISOF	Real	Iso-surface dump interval		s	Δt/NFRAMES
DT_MASS	Real	Mass diagnostic dump interval		s	Δt/NFRAMES
DT_PART	Real	Particle dump interval		s	Δt/NFRAMES
DT_PL3D	Real	PLOT3D dump interval		s	Δt/5
DT_PROF	Real	Profile dump interval		s	Δt/NFRAMES
DT_RESTART	Real	Restart core dump interval		s	1000000.
DT_SLCF	Real	Slice dump interval		s	Δt/NFRAMES
FLUSH_FILE_BUFFERS	Logical	See Section 14.1			.TRUE.
MASS_FILE	Logical	Flag for species MASS file			.FALSE.
MAXIMUM_DROPLETS	Integer	Max particles per mesh			500000
NFRAMES	Integer	Number of Frames of output data			1000
PLOT3D_QUANTITY(5)	Char. Quint	See Section 14.2.6			
PLOT3D_SPEC_ID(5)	Char. Quint	See Section 14.2.6			
SMOKE3D	Logical	Flag for 3D Smoke Visualization			.TRUE.
SMOKE3D_QUANTITY	Character	See Section 14.2.7			
SMOKE3D_SPEC_ID	Character	See Section 14.2.7			
STATE_FILE	Logical	Flag for state relation file			.FALSE.
STATUS_FILES	Logical	Flag for status (notready) file			.FALSE.
WRITE_XYZ	Logical	Flag for writing PLOT3D .xyz file			.FALSE.

Δt=T_END−T_BEGIN

15.6 HEAD (Header Parameters)

Table 15.6: For more information see Section 6.1.

HEAD (Header Parameters)				
CHID	Character	Job Identification String		'output'
FYI	Character	Comment String (has no effect)		
TITLE	Character	Title for job		

15.7 HOLE (Obstruction Cutout Parameters)

Table 15.7: For more information see Section 7.3.

HOLE (Obstruction Cutout Parameters)				
COLOR	Character	Color name of obstruction color		
CTRL_ID	Character	ID of ConTRoL to control hole's existence		
DEVC_ID	Character	ID of DEViCe to control hole's existence		

HOLE (Obstruction Cutout Parameters)				
`FYI`	Character	Comment String (has no effect)		
`RGB(3)`	Integer Triplet	Color indices (0 - 255) for resulting obstruction(s)		
`TRANSPARENCY`	Real	Transparency of obstruction		
`XB(6)`	Real Sextuplet	Physical coordinates	m	

15.8   `INIT` **(Initial Conditions)**

Table 15.8: For more information see Section 6.5.

INIT (Initial Conditions)				
`DENSITY`	Real	Initial value of density	kg/m^3	Ambient
`MASS_FRACTION(II)`	Real Array	Initial value of species `II`	kg/kg	Ambient
`TEMPERATURE`	Real	Initial value of temperature	°C	`TMPA`
`XB(6)`	Real Sextuplet	Coordinates	m	

15.9   `ISOF` **(Isosurface Parameters)**

Table 15.9: For more information see Section 14.2.5.

ISOF (Isosurface Parameters)				
`FYI`	Character	Comment String (has no effect)		
`QUANTITY`	Character	Quantity to visualize		
`SPEC_ID`	Character	Species indicator (if needed)		
`VALUE(I)`	Real Array	Contour value(s)		

15.10   `MATL` **(Material Properties)**

Table 15.10: For more information see Section 8.2.

MATL (Material Properties)				
`A`	Real array	Pre-exponential factors	1/s	
`ABSORPTION_COEFFICIENT`	Real	Absorption Coefficient	1/m	50000.
`BOILING_TEMPERATURE`	Real	Boiling temperature	°C	5000.
`CONDUCTIVITY`	Real	Thermal conductivity	W/m/K	0.
`CONDUCTIVITY_RAMP`	Character	Ramp ID for conductivity		
`DENSITY`	Real	Solid mass per unit volume	kg/m^3	0.
`E`	Real array	Activation energies	kJ/kmol	
`EMISSIVITY`	Real	Emissivity		0.9

MATL (Material Properties)				
FYI	Character	Comment String (has no effect)		
HEATING_RATE	Real array	See Section 8.3.2	°C/min	5.
HEAT_OF_COMBUSTION(:,II)	Real array	Heats of combustion for species II	kJ/kg	0.
HEAT_OF_REACTION(:)	Real array	Heats of reaction	kJ/kg	0.
INITIAL_VAPOR_FLUX	Real	Initial evaporation rate	$m^2/(sm^2)$	0.0005
ID	Character	IDentifier		
THRESHOLD_TEMPERATURE	Real array	See Section 8.3.2	°C	-273.15
N_REACTIONS	Character	Number of Reactions		0
N_S	Real array	See Section 8.3.2		1.
N_T	Real array	See Section 8.3.2		0.
NU_FUEL	Real array	Fuel gas yields	kg/kg	0.
NU_GAS(:,II)	Real array	Yields of species II	kg/kg	0.
NU_RESIDUE	Real array	Residue yields	kg/kg	0.
NU_WATER	Real aray	Water vapor yields	kg/kg	0.
PYROLYSIS_RANGE	Real array	See Section 8.3.2	°C	80.
REFERENCE_TEMPERATURE	Real array	See Section 8.3.2	°C	
RESIDUE	Character	IDs of residue MATL		
SPECIFIC_HEAT	Real	Specific heat	kJ/kg/K	0.
SPECIFIC_HEAT_RAMP	Character	Ramp ID for specific heat		

15.11 MESH (Mesh Parameters)

Table 15.11: For more information see Section 6.3.

MESH (Mesh Parameters)				
COLOR	Character	Mesh Line Color		'BLACK'
CYLINDRICAL	Logical	2-D Axi-symmetric calculation		.FALSE.
ID	Character	MESH IDentifier		
IJK	Integer Triplet	No. cells in *x*, *y*, and *z* directions		10
FYI	Character	Comment String (has no effect)		
MPI_PROCESS	Integer	See Section 6.3.3		
RGB	Integer Triplet	Color indices (0-255)		0,0,0
SYNCHRONIZE	Logical	Sync. time steps of multiple meshes		.TRUE.
XB(6)	Real Sextuplet	Min/Max Coordinates of the MESH	m	0,1,0,1,0,1

15.12 MISC (Miscellaneous Parameters)

Table 15.12: For more information see Section 6.4.

MISC (Miscellaneous Parameters)				
ALLOW_UNDERSIDE_DROPLETS	Logical	See Section 12.2		.FALSE.
ASSUMED_GAS_TEMPERATURE	Real	See Section 8.4		
BACKGROUND_SPECIES	Character	See Section 11.2		'AIR'
BAROCLINIC	Logical	Baroclinic torque correction		.FALSE.
BNDF_DEFAULT	Logical	See Section 14.2.4		.TRUE.
CFL_MAX	Real	See Section 6.4.8		1.0
CFL_MIN	Real	See Section 6.4.8		0.8
CSMAG	Real	Smagorinsky constant		0.20
CONDUCTIVITY	Real	See Section 11.2	W/m/K	
CO_PRODUCTION	Logical	See Section 11.1.2		.FALSE.
DNS	Logical	Direct Numerical Simulation		.FALSE.
FYI	Character	Comment String (has no effect)		
GROUND_LEVEL	Real	See Section 9.4	m	0.
GVEC	Real triplet	Gravity vector	m/s^2	0,0,-9.81
H_FIXED	Real	See Section 8.4	W/m^2/K	
HUMIDITY	Real	Relative Humidity	%	40.
ISOTHERMAL	Logical	Isothermal calculation		.FALSE.
LAPSE_RATE	Real	See Section 9.4	°C/m	0
LES	Logical	Large Eddy Simulation		.TRUE.
MW	Real	Molecular Weight (Section 11.2)	g/mol	
NOISE	Logical	Toggle initial noise on and off		.TRUE.
PR	Real	Prandtl number (LES only)		0.5
P_INF	Real	Ambient pressure	Pa	101325
POROUS_FLOOR	Logical	See Section 13.3.1		.TRUE.
PRESSURE_CORRECTION	Logical	See Section 6.4.4		.FALSE.
RADIATION	Logical	Radiation calculation flag		.TRUE.
RAMP_GX	Character	Time function, x comp. of gravity		
RAMP_GY	Character	Time function, y comp. of gravity		
RAMP_GZ	Character	Time function, z comp. of gravity		
RESTART	Logical	Restart previous calculation		.FALSE.
RESTART_CHID	Character	Restart file CHID		CHID
SC	Real	Schmidt number (LES only)		0.5
SOLID_PHASE_ONLY	Logical	See Section 8.4		.FALSE.
STRATIFICATION	Logical	See Section 9.4		.TRUE.
SUPPRESSION	Logical	See Section 11.1.2		.TRUE.
SURF_DEFAULT	Character	Default SURFace type		'INERT'
TEXTURE_ORIGIN(3)	Char. Triplet	See Section 7.5.1	m	(0.,0.,0.)
THICKEN_OBSTRUCTIONS	Logical	See Section 7.2		.FALSE.
TMPA	Real	Ambient Temperature	°C	20.
U0,V0,W0	Reals	Prevailing velocity field	m/s	0.
VISCOSITY	Real	See Section 11.2	kg/m/s	
VN_MAX	Real	See Section 6.4.8		1.0
VN_MIN	Real	See Section 6.4.8		0.8

15.13 `MULT` (Multiplier Function Parameters)

Table 15.13: For more information see Section 7.2.2.

MULT (Multiplier Function Parameters)				
DXB	Real Sextuplet	Spacing for all 6 coordinates	m	0.
DX	Real	Spacing in the x direction	m	0.
DY	Real	Spacing in the y direction	m	0.
DZ	Real	Spacing in the z direction	m	0.
DX0	Real	Translation in the x direction	m	0.
DY0	Real	Translation in the y direction	m	0.
DZ0	Real	Translation in the z direction	m	0.
ID	Character	IDentifier		
I_LOWER	Integer	Lower array bound, x direction		0
I_UPPER	Integer	Upper array bound, x direction		0
J_LOWER	Integer	Lower array bound, y direction		0
J_UPPER	Integer	Upper array bound, y direction		0
K_LOWER	Integer	Lower array bound, z direction		0
K_UPPER	Integer	Upper array bound, z direction		0
N_LOWER	Integer	Lower sequence bound		0
N_UPPER	Integer	Upper sequence bound		0

15.14 `OBST` (Obstruction Parameters)

Table 15.14: For more information see Section 7.2.

OBST (Obstruction Parameters)				
ALLOW_VENT	Logical	Allow vents on obstruction		.TRUE.
BNDF_FACE(-3:3)	Logical Array	See Section 14.2.4		.TRUE.
BNDF_OBST	Logical	See Section 14.2.4		.TRUE.
BULK_DENSITY	Real	See Section 8.3.4		1
COLOR	Character	Color name of obstruction color		
CTRL_ID	Character	ID of Controlling ConTRoL		
DEVC_ID	Character	ID of Controlling DEViCe		
FYI	Character	Comment String (has no effect)		
OUTLINE	Logical	Draw as Outline		.FALSE.
PERMIT_HOLE	Logical	Allow a Hole		.TRUE.
REMOVABLE	Logical	Allow obstruction to be removed		.TRUE.
RGB(3)	Integer Triplet	Color indices (0 - 255)		
SAWTOOTH	Logical	See Section 7.2.3		.TRUE.
SURF_ID	Character	Associated Surface		
SURF_IDS(3)	Character Triplet	Associated Surfaces (top,side,bot.)		
SURF_ID6(6)	Character Sextuplet	Associated Surfaces (like XB)		
THICKEN	Logical	Force at least one cell thick		.FALSE.

OBST (Obstruction Parameters)				
`TEXTURE_ORIGIN(3)`	Real Triplet	See Section 7.5.1	m	(0.,0.,0.)
`TRANSPARENCY`	Real	Transparency indicator		1
`XB(6)`	Real Sextuplet	Min/Max Physical coordinates	m	

15.15 `PART` (Lagrangian Particles/Droplets)

Table 15.15: For more information see Section 12.

PART (Lagrangian Particles/Droplets)				
`AGE`	Real	Droplet lifetime	s	100000.
`COLOR`	Character	Default color of droplets		'BLACK'
`DENSITY`	Real	Droplet density	kg/m^3	1000.
`DIAMETER`	Real	Median Volumetric Diameter	μm	500.
`DROPLETS_PER_SECOND`	Integer	Drops per second per head		5000
`DT_INSERT`	Real	Time between insertions	s	0.01
`EVAPORATE`	Logical	Assume liquid evaporation		.TRUE.
`FYI`	Character	Comment String		
`FUEL`	Logical	Liquid Fuel		.FALSE.
`GAMMA_D`	Real	Size distribution parameter		2.4
`HEAT_OF_COMBUSTION`	Real	Heat of Combustion	kJ/kg	
`HEAT_OF_VAPORIZATION`	Real	Latent Heat of Vaporization	kJ/kg	
`H_V_REFERENCE_TEMPERATURE`	Real	Temperature for Heat of Vaporization	°C	0.
`HORIZONTAL_VELOCITY`	Real	Droplet speed, horizontal	m/s	0.2
`ID`	Character	Identifier		
`INITIAL_TEMPERATURE`	Real	Initial Temperature	°C	TMPA
`MASSLESS`	Logical	Massless tracers		.FALSE.
`MASS_PER_VOLUME`	Real	Mass per unit volume	kg/m^3	1.
`MAXIMUM_DIAMETER`	Real	Break-up bound	μm	∞
`MINIMUM_DIAMETER`	Real	Evaporation bound	μm	20.
`MELTING_TEMPERATURE`	Real	Melting Temperature	°C	0.
`MONODISPERSE`	Logical	Uniform droplet size		.FALSE.
`NUMBER_INITIAL_DROPLETS`	Integer	Number of droplets at start		0
`QUANTITIES(10)`	Character	Quantities for coloring		
`RGB(3)`	Integers	Color indices (0-255)		
`SAMPLING_FACTOR`	Integer	Filter for output file		1
`SIGMA_D`	Real	Size distribution parameter		
`SPEC_ID`	Character	Name of gas species		
`SPECIFIC_HEAT`	Real	Droplet specific heat	kJ/kg/K	4.184
`STATIC`	Logical	Stationary Particles		.FALSE.
`VAPORIZATION_TEMPERATURE`	Real	Liquid Droplet Boiling Temp	°C	100.
`VERTICAL_VELOCITY`	Real	Droplet speed, vertical	m/s	0.5
`XB(6)`	Real array	Initial particle location	m	

PART (Lagrangian Particles/Droplets)				
WATER	Logical	Water Droplet		.FALSE.

15.16 PROF (Wall Profile Parameters)

Table 15.16: For more information see Section 14.2.2.

PROF (Wall Profile Parameters)				
IOR	Real	Orientation of wall surface		
ID	Character	Identifier		
FYI	Character	Comment String (has no effect)		
QUANTITY	Character	Name of output quantity		
XYZ	Real Triplet	Coordinates of wall surface	m	

15.17 PROP (Device Properties)

Table 15.17: For more information see Section 13.3.

PROP (Device Properties)				
ACTIVATION_TEMPERATURE	Real	Threshold link temperature	°C	74
ACTIVATION_OBSCURATION	Real	Threshold value of obscuration	%/m	3.28
ALPHA_C	Real	Smoke detector parameter		1.8
ALPHA_E	Real	Smoke detector parameter		0.0
BETA_C	Real	Smoke detector parameter		1.0
BETA_E	Real	Smoke detector parameter		1.0
BEAD_DIAMETER	Real	Diameter of TC bead	m	0.001
BEAD_EMISSIVITY	Real	Emissivity of TC bead		0.85
CABLE_DIAMETER	Real	See Section 13.3.7	m	0.02
CABLE_FAILURE_TEMPERATURE	Real	See Section 13.3.7	°C	400
CABLE_JACKET_THICKNESS	Real	See Section 13.3.7	m	0.002
CABLE_MASS_PER_LENGTH	Real	See Section 13.3.7	kg/m	0.5
C_FACTOR	Real	Sprinkler activation parameter		0.
CHARACTERISTIC_VELOCITY	Real	See Section 14.3.12	m/s	1.0
DROPLET_VELOCITY	Real	Initial droplet velocity	m/s	0.0
FLOW_RATE	Real	Sprinkler or nozzle flow rate	L/min	
FLOW_RAMP	Character	Time RAMP for flow		
FLOW_TAU	Real	Time constant for flow		0.0
GAUGE_TEMPERATURE	Real	See Section 14.3.5	°C	TMPA
ID	Character	IDentifier		
INITIAL_TEMPERATURE	Real	Initial link temperature	°C	TMPA
K_FACTOR	Real	Flow parameter	$L/min/atm^{1/2}$	1.

PROP (Device Properties)					
LENGTH	Real	Smoke detector parameter			1.8
OFFSET	Real	Droplet offset distance	m		0.05
OPERATING_PRESSURE	Real	Sprinkler pipe pressure	atm		1.
ORIFICE_DIAMETER	Real	Nozzle orifice diameter	m		0.0
PART_ID	Character	Name of associated PART line			
PDPA_END	Real	See Section 14.3.6	s		T_END
PDPA_M	Integer	See Section 14.3.6			0
PDPA_M	Integer	See Section 14.3.6			0
PDPA_RADIUS	Real	See Section 14.3.6	m		0.1
PDPA_START	Real	See Section 14.3.6	s		0.
PRESSURE_RAMP	Character	Pressure RAMP for sprinkler systems			
QUANTITY	Character	Name of associated output			
RTI	Real	Response Time Index	$\sqrt{m\,s}$		100.
SMOKEVIEW_ID	Character	Name of drawn object			
SPEC_ID	Character	See Section 13.3.4			
SPRAY_ANGLE(2)	Real	Cone angles for water spray	deg		60.,75.
SPRAY_PATTERN_TABLE	Character	TABL for spray pattern			

15.18 RADI (Radiation Parameters)

Table 15.18: For more information see Section 11.3.

RADI (Radiation Parameters)					
ANGLE_INCREMENT	Integer	Number of angles skipped per update			5
CH4_BANDS	Logical	Include extra fuel bands			.FALSE.
KAPPA0	Real	Constant absorption coefficient	1/m		0
NMIEANG	Integer	Number of polar angles			15
NUMBER_RADIATION_ANGLES	Integer	Number of solid angles			104
PATH_LENGTH	Real	Path length for radiation calc.	m		
RADIATIVE_FRACTION	Real	Radiative Loss Fraction			0.35
RADTMP	Real	Assumed radiative source temp.	°C		900
TIME_STEP_INCREMENT	Integer	Number time steps skipped			3
WIDE_BAND_MODEL	Logical	Non-gray gas assumption			.FALSE.

15.19 RAMP (Ramp Function Parameters)

Table 15.19: For more information see Section 10.

RAMP (Ramp Function Parameters)				
FYI	Character	Comment String (has no effect)		

RAMP (Ramp Function Parameters)				
F	Real	Function value		
FYI	Character	Comment String (has no effect)		
ID	Character	Identifier		
T	Real	Time (or Temperature)	s (or °C)	
X	Real	x-coordinate (gravity only)	m	

15.20 REAC (Reaction Parameters)

Table 15.20: For more information see Section 11.1.

REAC (Reaction Parameters)				
BOF	Real	Pre-exponential Factor (Finite Rate)	cm^3/mol/s	
C	Real	Carbon atoms in fuel		3
C_EDC	Real	See Section 11.1.5		0.1
CO_YIELD	Real	Fraction of CO from the fuel	kg/kg	0
CRITICAL_FLAME_TEMPERATURE	Real	Suppression criterion	°C	1427
E	Real	Activation Energy (Finite Rate)	kJ/kmol	
EDDY_DISSIPATION	Logical	See Section 11.1.5		.TRUE.
EPUMO2	Real	Energy per Unit Mass Oxygen	kJ/kg	13100
FUEL	Character	Name of Fuel (Finite Rate)		
FYI	Character	Comment String (has no effect)		
H	Real	Hydrogen atoms in fuel		8
H2_YIELD	Real	Fraction of H$_2$ from the fuel	kg/kg	0
HEAT_OF_COMBUSTION	Real	Energy per Unit Mass Fuel	kJ/kg	
HRRPUA_SHEET	Real	See Section 11.1.5	kW/m^2	200.
HRRPUV_AVERAGE	Real	See Section 11.1.5	kW/m^3	3000.
HRRPUV_AVERAGE_TIME	Real	See Section 11.1.5	s	1.
ID	Character	Identifier		
IDEAL	Logical	Adjust for minor product yields		.FALSE.
MASS_EXTINCTION_COEFFICIENT	Real	Visibility parameter	m^2/kg	8700.
MAXIMUM_VISIBILITY	Real	Visibility parameter	m	30
MW_OTHER	Real	Molecular Weight of OTHER	g/mol	28
N	Real	Nitrogen atoms in the fuel		0
N_S(N)	Real	Arrhenius Exponents (Finite Rate)		
NU(N)	Real	Reaction stoichiometry (Finite Rate)		
O	Real	Oxygen atoms in the fuel		0
OTHER	Real	Other atoms in the fuel		0
OXIDIZER	Character	Name of Oxidizer (Finite Rate)		
SOOT_YIELD	Real	Fraction of soot from the fuel	kg/kg	0.01
SOOT_H_FRACTION	Real	Atom fraction of hydrogen in soot		0.1
VISIBILITY_FACTOR	Real	Visibility parameter		3
X_O2_LL	Real	Lower Oxygen Limit	mol/mol	0.15

REAC (Reaction Parameters)				
Y_F_INLET	Real	Mass Frac. of Fuel in Burner	kg/kg	1.0
Y_F_LFL	Real	Lower Fuel limit (mass fraction)	kg/kg	0.0
Y_O2_INFTY	Real	Ambient oxygen mass fraction	kg/kg	0.23

15.21 SLCF (Slice File Parameters)

Table 15.21: For more information see Section 14.2.3.

SLCF (Slice File Parameters)				
CELL_CENTERED	Logical	Show raw data with no averaging		.FALSE.
FYI	Character	Comment String (has no effect)		
MESH_NUMBER	Integer	Save only slices in this mesh		
PART_ID	Character	Particle identifier (if needed)		
PBX	Real	x-plane to save slice file		
PBY	Real	y-plane to save slice file		
PBZ	Real	z-plane to save slice file		
QUANTITY	Character	Name of Quantity to display		
SPEC_ID	Character	Species identifier (if needed)		
VECTOR	Logical	Include flow vectors		.FALSE.
XB(6)	Real Sextuplet	Min/Max coordinates of region to save	m	

15.22 SPEC (Species Parameters)

Table 15.22: For more information see Section 11.2.

SPEC (Species Parameters)				
ABSORBING	Logical	Absorbs radiation		.FALSE.
CONDUCTIVITY	Real	Conductivity k	W/m/K	
DIFFUSIVITY	Real	Diffusivity D	m^2/s	
EPSILONKLJ	Real	Leonard-Jones Parameter		0
FORMULA	Character	Chemical formula for Smokeview label		
FYI	Character	Comment String		
ID	Character	Name of species		
MASS_EXTINCTION_COEFFICIENT	Real	See Section 13.3.4		0
MASS_FRACTION_0	Real	Initial mass fraction		0
MW	Real	Molecular Weight	g/mol	29.
REFERENCE_TEMPERATURE	Real	Temperature for Specific Enthalpy	°C	25.
SPECIFIC_ENTHALPY	Real	Specific Enthalpy	kJ/kg	

SPEC (Species Parameters)				
SPECIFIC_HEAT	Real	Specific Heat	kJ/kg/K	
SIGMALJ	Real	Leonard-Jones Parameter		0
VISCOSITY	Real	Dynamic Viscosity *mu*	kg/m/s	

15.23 SURF (**Surface Properties**)

Table 15.23: For more information see Section 7.1.

SURF (Surface Properties)				
ADIABATIC	Logical	Adiabatic thermal BC		.FALSE.
BACKING	Character	Back boundary condition		'VOID'
BURN_AWAY	Logical	See Section 8.3.4		.FALSE.
CELL_SIZE_FACTOR	Real	See Section 8.2.7		1.0
COLOR	Character	Surface Color		
CONVECTIVE_HEAT_FLUX	Real	Heat flux at surface	kW/m^2	0.
DUCT_PATH	Int. Pair	Pressure Zones for fans		0,0
E_COEFFICIENT	Real	Extinguishing coefficient	m^2/kg/s	0.
EMISSIVITY	Real	Emissivity		0.9
EXTERNAL_FLUX	Real	Heat flux to surface	kW/m^2	0.
FREE_SLIP	Logical	See Section 9.5		.FALSE.
FYI	Character	Comment String		
GEOMETRY	Character	Geometry type		'CARTESIAN'
HEAT_OF_VAPORIZATION	Real	For specified HRR only	kJ/kg	0.
HRRPUA	Real	HRR Per Unit Area	kW/m^2	0.
ID	Character	IDentifier		
IGNITION_TEMPERATURE	Real	Ignition temperature	°C	5000.
LAYER_DIVIDE	Real	See Section 8.2.5		0.5 × n.of.layers
LEAK_PATH	Int. Pair	Pressure Zones for leakage		
MASS_FLUX(I)	Real Array	For species I	kg/m^2 s	0.
MASS_FLUX_TOTAL	Real	Total Mass Flux	kg/m^2 s	
MASS_FRACTION(I)	Real Array	For species I		
MATL_ID	Char. Array	(Layer,Component)		
MATL_MASS_FRACTION	Real Array	(Layer,Component)		
MAX_PRESSURE	Real	Max over-pressure for fan	Pa	1.E12
MLRPUA	Real	Mass loss rate per unit area	kg/m^{2}s	0.
NET_HEAT_FLUX	Real	Net flux at surface	kW/m^2	0.
NO_SLIP	Logical	See Section 9.5		.FALSE.
NPPC	Integer	Number of particles per cell		1
PARTICLE_MASS_FLUX	Real	See Section 12.2.2	kg/m^2 s	0.
PART_ID	Character	Lagrangian Particle ID		
POROUS	Logical	See Section 9.1		.FALSE.
PLE	Real	Atmospheric profile exp.		0.3

SURF (Surface Properties)				
PROFILE	Character	Name of velocity profile		
RAMP_MF(I)	Character	Ramp ID for species I		
RAMP_Q	Character	Ramp ID for HRR		
RAMP_T	Character	Ramp ID for temp.		
RAMP_V	Character	Ramp ID for velocity		
RGB(3)	Int. Triplet	Color indices (0-255)		255,204,102
SHRINK	Logical	Shrinking material		.TRUE.
STRETCH_FACTOR	Real	See Section 8.2.7		2.0
SURFACE_DENSITY	Real	See Section 8.3.4	kg/m^2	0.0
TAU_MF(I)	Real Array	Ramp time for species I	s	1.
TAU_Q	Real	Ramp time for HRR	s	1.
TAU_T	Real	Ramp time for temp.	s	1.
TAU_V	Real	Ramp time for velocity	s	1.
TEXTURE_HEIGHT	Real	Height of texture image	m	1.
TEXTURE_MAP	Character	Name of texture map file		
TEXTURE_WIDTH	Real	Width of texture image	m	1.
THICKNESS(IL)	Real Array	Thickness of Layer IL	m	0.
TMP_BACK	Real	Back surface temperature BC	°C	20.
TMP_FRONT	Real	Front surface temperature	°C	20.
TMP_INNER	Real	Initial solid temperature	°C	20.
TRANSPARENCY	Real	Transparency of obstruction	1	
VEL	Real	Normal velocity	m/s	0.
VEL_T	Real Pair	Tangential velocity comps.	m/s	0.
VOLUME_FLUX	Real	Normal velocity x vent area	m^3/s	0.
Z0	Real	Atmospheric profile origin	m	10.

15.24 TABL (Table Parameters)

Table 15.24: For more information see Section 10.

TABL (Table Parameters)				
ID	Character	IDentifier		
FYI	Character	Comment String (has no effect)		
TABLE_DATA	Real Array	Data for one row of the table		

15.25 TIME (Time Parameters)

TIME (Time Parameters)				
DT	Real	Initial time step	s	
FYI	Character	Comment String (has no effect)		
LOCK_TIME_STEP	Logical	Do not allow time step changes		.FALSE.
RESTRICT_TIME_STEP	Logical	Do not allow time step to exceed initial		.TRUE.
SYNCHRONIZE	Logical	Sync time step of multiple meshes		.TRUE.
T_BEGIN	Real	Starting time for calculation	s	0.
T_END (TWFIN)	Real	Ending time for calculation	s	1
TIME_SHRINK_FACTOR	Real	See Section 6.2.3		1.
WALL_INCREMENT	Integer	Time steps between 1D wall solution updates		2

15.26 TRNX, TRNY, TRNZ (MESH Transformations)

Table 15.26: For more information see Section 6.3.5.

TRNX, TRNY, TRNZ (MESH Transformations)				
CC	Real	Computational coordinate	m	
FYI	Character	Comment String (has no effect)		
IDERIV	Integer	Order of polynomial transformation		
MESH_NUMBER	Integer	Number of mesh to transform		
PC	Real	Physical coordinate or derivative		

15.27 VENT (Vent Parameters)

Table 15.27: For more information see Section 7.4.

VENT (Vent Parameters)				
COLOR	Character	See Section 7.5		
CTRL_ID	Character	ID of Control Function		
DEVC_ID	Character	ID of Controlling Device		
DYNAMIC_PRESSURE	Real	See Section 9.3	Pa	0.0
FYI	Character	Comment String (has no effect)		
IOR	Integer	Orientation Index		
MASS_FRACTION(N)	Real Array	Mass Fraction of species N at OPEN vent	kg/kg	
MB	Character	Mesh Boundary		
OUTLINE	Logical	Draw vent as outline		.FALSE.
PBX, PBY, PBZ	Real	Coordinate Plane		
PRESSURE_RAMP	Character	See Section 9.3		
RGB(3)	Integer Triplet	See Section 7.5		
SPREAD_RATE	Real	See Section 8.1.3	m/s	0.0
SURF_ID	Character	Associated Surface		'INERT'

VENT (Vent Parameters)				
TEXTURE_ORIGIN(3)	Real Triplet	See Section 7.5.1	m	(0.,0.,0.)
TMP_EXTERIOR	Real	Temperature at OPEN vent	°C	
TRANSPARENCY	Real	Transparency indicator		1.0
XB(6)	Real Sextuplet	Min/Max physical coordinates	m	
XYZ(3)	Real Triplet	See Section 8.1.3	m	

15.28 ZONE **(Pressure Zone Parameters)**

Table 15.28: For more information see Section 9.6.

ZONE (Pressure Zone Parameters)				
ID	Character	IDentifier		
LEAK_AREA(N)	Real	Leakage area to pressure zone N	m^2	0
XB(6)	Real Sextuplet	Coordinates of Zone	m	

Chapter 16

Conversion of Old Input Files to FDS 5

Many changes and improvements have been made in the latest release FDS 5. To make an FDS 4 input data file compatible with the new FDS 5 application, a few changes must be made to the file. This appendix will point out all the changes that need to be made to convert an FDS 4.x input file to the new FDS 5.x format.

16.1 Numerical Domain Parameters: `GRID` and `PDIM`

In previous versions, the computational domain and numerical mesh were specified via lines of the form:

```
&GRID IBAR=30, JBAR=20, KBAR=10 /
&PDIM XBAR0=0.0, XBAR=3.0, YBAR0=0.0, YBAR=2.0, ZBAR0=0.0, ZBAR=1.0 /
```

In FDS 5, these two lines are now written via the single line:

```
&MESH IJK=30,20,10, XB=0.0,3.0,0.0,2.0,0.0,1.0 /
```

Rules for multiple meshes and mesh transformations still apply.

16.2 Obstructions, Vents, and Holes: `OBST`, `VENT`, and `HOLE`

The syntax for these lines is fairly similar to past versions, with the following exceptions:

- For a `VENT` that spans an entire mesh boundary, `CB='XBAR0'` is now `MB='XMIN'`. The character string `'XBAR'` is now `'XMAX'`. The same applies for the *y* and *z* coordinate parameters.

- Control parameters like `T_ACTIVATE`, `HEAT_REMOVE`, *etc.*, are now consolidated into `DEVC_ID` and `CTRL_ID`. In brief, any change to an obstruction, vent, or hole is tied to a specific device or control function. See Sections 13.1 and 13.5 for details.

16.3 Surface Parameters: `SURF`

The most significant change to the input file format has been splitting of the `SURF` line. In past versions, the `SURF` namelist group contained all the information about a particular boundary type – its material properties, color, thickness, and so on. However, in FDS 5, solid boundaries can now consist of multiple layers of materials, making the old `SURF` line too cumbersome to specify. Instead, there is a new namelist group called `MATL` that just contains the properties of a given material. What used to be

```
&SURF ID       = 'BRICK WALL'
     RGB       = 0.6,0.2,0.2
     KS        = 0.69
     C_P       = 0.84
     DENSITY   = 1600.
     BACKING   = 'EXPOSED'
     THICKNESS = 0.20 /
```

is now given by two input lines:

```
&MATL ID            = 'BRICK'
     CONDUCTIVITY   = 0.69
     SPECIFIC_HEAT  = 0.84
     DENSITY        = 1600. /

&SURF ID       = 'BRICK WALL'
     MATL_ID   = 'BRICK'
     RGB       = 166,41,41
     BACKING   = 'EXPOSED'
     THICKNESS = 0.20 /
```

The surface is still specified the same way as before, for example:

```
&OBST XB=0.1, 5.0, 1.0, 1.2, 0.0, 1.0, SURF_ID='BRICK WALL' /
```

Notice the change in the names of the thermal properties KS and C_P to CONDUCTIVITY and SPECIFIC_HEAT, respectively. Notice that the color RGB is now specified via integers between 0 and 255, instead of real numbers between 0.0 and 1.0. Better yet, just use the COLOR Table 7.1.

16.4 Reaction Parameters: REAC

For most applications, the specification of the combustion reaction has become easier. In past versions, you needed to specify the fuel, its molecular weight, soot and/or CO yields, and the ideal stoichiometry of the reaction:

```
&REAC ID             = 'PROPANE'
     FYI             = 'C_3 H_8'
     MW              = 44.
     SOOT_YIELD      = 0.01
     NU_O2           = 5.
     NU_CO2          = 3.
     NU_H2O          = 4. /
```

Now, you just need to describe the composition of the fuel molecule and any non-ideal product yield. FDS 5 computes what it needs based on this information.

```
&REAC ID             = 'PROPANE'
     SOOT_YIELD      = 0.01
     C               = 3.
     H               = 8. /
```

16.5 Device Parameters: SPRK, SMOD, HEAT, THCP

Past versions of FDS had a variety of ways to specify devices. For example, a sprinkler was specified via a line of the form:

```
&SPRK XYZ=4.5,6.7,3.6, MAKE='Acme_K-17', LABEL='spk_34' /
```

which located the sprinkler at XYZ and indicated that the sprinkler's properties were listed in a file called **Acme_K-17.spk**. Smoke and heat detectors were specified via lines of the form:

```
&SMOD XYZ=4.5,6.7,3.6, LENGTH=2.6, ACTIVATION_OBSCURATION=1.4, LABEL='sd_34' /
&HEAT XYZ=4.5,6.7,3.6, RTI=45., ACTIVATION_TEMPERATURE=74., LABEL='hd_39' /
```

In FDS 5, these devices are all specified in the same way:

```
&PROP ID='Acme_K-17', QUANTITY='SPRINKLER LINK TEMPERATURE', RTI=148., C_FACTOR=0.7,
      ACTIVATION_TEMPERATURE=74., PART_ID='water drops', FLOW_RATE=189.3,
      DROPLET_VELOCITY=10., SPRAY_ANGLE=30.,80.   /

&DEVC ID='spk_34', XYZ=4.5,6.7,3.6, PROP_ID='Acme_K-17' /
```

Point output via "thermocouples" (THCPs) are now given by "devices" (DEVCs):

```
&DEVC XYZ=0.7,0.9,2.1, QUANTITY='WALL TEMPERATURE', IOR=-2, ID='probe_2' /
```

The syntax of the old THCP namelist group is almost the same. Just swap DEVC for THCP, and change LABEL to ID. In FDS 5, any input record is identified via its ID.

Part III

FDS and Smokeview Development Tools

Chapter 17

The FDS/Smokeview Repository

For those interested in obtaining the FDS and Smokeview source codes, either for development work or simply to compile on a particular platform, it is strongly suggested that you download onto your computer the entire FDS/Smokeview "Repository." All project documents are maintained using the online utility Google Code Project Hosting, a free service offered by Google to support software development for open source applications. Google Code uses the Subversion (SVN) revision management system. Under this system a centralized repository containing all project files resides on a Google Code server. Subversion uses a single integer that identifies the version of the entire repository rather than of a specific file (i.e. anytime a change is made to the repository all files are incremented in version number). A record of version number when a specific file was last changed is maintained.

As an open source program, any individual can obtain a copy of the repository or retrieve specific versions repository. Only the FDS and Smokeview developers can commit changes to the repository.

The current location of the FDS repository is http://fds-smv.googlecode.com/svn/trunk/. The repository contains the following files:

1. FDS and Smokeview source code files

2. FDS and Smokeview documentation

3. Input files for software testing (Examples), verification testing, and validation testing

4. Experimental data files used for validation testing

5. Scripts and post-processing utilities used for software testing

6. Web pages and wikis

The wikis are particularly useful in describing the details of how you go about working with the Repository assets.

Chapter 18

Compiling FDS

This section describes what you need to know if you want to compile the FDS source code yourself. It is not a step by step guide, more detailed instructions can be found on Developer section of the web site at http://fire.nist.gov/fds.

If a compiled version of FDS exists for the machine on which the calculation is to be run and no changes have been made to the original source code, there is no need to re-compile the code. For example, the file **fds5.exe** is the compiled single processor program for a Windows-based PC; thus PC users do not need a Fortran compiler and do not need to compile the source code. For machines for which an executable has not been compiled, you must compile the code. Fortran 90/95 and C compilers are needed for compilation.

18.1 FDS Source Code

Table 18.1 lists the files that make up the source code. The files with suffix ".f90" contain free form Fortran 90 instructions conforming to the ANSI and ISO standards, with a few exceptions that are discussed below. The source files should be compiled in the order in which they are listed in Table 18.1 because some routines are dependent on others. For Unix/Linux users, **Makefiles** for various platforms are available that assist in the compilation. Compiler options differ from platform to platform. Note the following:

- The source code consists mainly of Fortran 90 statements organized into about 25 files, plus an extra file containing some additional C routines needed for output to Smokeview. All of the C code is contained within the file called **isob.c**.

- Be aware that different compilers handle the names of C subroutines differently. Some compilers append an underscore to the names of the C routines called by the Fortran code. If the compiler produces an error involving the names of routines that are not recognized, invoke the C compiler pre-processing directive `pp_noappend` to stop the compiler from appending the underscore to the names of the C routines.

- There is only one non-standard call in the Fortran code. The non-standard call is `GETARG`, in **func.f90**. This routine reads the name of the input file off of the command line. This call cannot be simply commented out; a suitable alternative must be found. The only compiler option necessary, in addition to any needed to address the above issues, is for full optimization (usually -O or some variant). Some compilers have a standard optimization level, plus various degrees of "aggressive" optimization. Be cautious in using the highest levels of optimization.

- For the single processor version of FDS, compile with **main.f90**

- The parallel version of FDS uses **main_mpi.f90** instead of **main.f90**, plus additional MPI libraries need to be installed. More details on MPI can be found at the web site, along with links to the necessary organizations who have developed free MPI libraries.

Table 18.1: **Source Code Files**

File Name	Description
isob.c	C Routine for computing isosurfaces and 3D smoke
prec.f90	Specification of numerical precision
smvv.f90	Interfaces for C routines used for Smokeview output
devc.f90	Derived type definitions and constants for devices'
type.f90	Derived type definitions
mesh.f90	Arrays and constants associated with each mesh
cons.f90	Global arrays and constants
func.f90	Global functions and subroutines
irad.f90	Functions needed for radiation solver, including RadCal
ieva.f90	Support routines for evac.f90
evac.f90	Egress computations (future capability)
pois.f90	Poisson (pressure) solver
radi.f90	Radiation solver
part.f90	Lagrangian particle transport and sprinkler activation
ctrl.f90	Definitions and routines for control functions
dump.f90	Output data dumps into files
read.f90	Read input parameters
mass.f90	Mass equation(s) and thermal boundary conditions
wall.f90	Wall boundary conditions
fire.f90	Combustion routines
pres.f90	Spatial discretization of pressure (Poisson) equation
divg.f90	Compute the flow divergence
init.f90	Initialize variables and Poisson solver
turb.f90	Experimental routines, mostly involving the turbulence model
velo.f90	Momentum equations
vege.f90	Experimental vegetation model
main.f90 **or** main_mpi.f90	Main programs, serial and parallel versions

Chapter 19

Output File Formats

The output from the code consists of the file **CHID.out**, plus various data files that are described below. Most of these output files are written out by the routine **dump.f**, and can easily be modified to accommodate various plotting packages.

19.1 Diagnostic Output

The file **CHID.out** consists of a list of the input parameters, and an accounting of various important quantities, including CPU usage. Typically, diagnostic information is printed out every 100 time steps

```
                         .
                         .

       Iteration   8300   May 16, 2003  08:37:53
       ----------------------------------------------
       Mesh  1, Cycle   3427
       CPU/step:     2.272 s, Total CPU:      2.15 hr
       Time step:  0.03373 s, Total time:   128.86 s
       Max CFL number: 0.86E+00 at ( 21,  9, 80)
       Max divergence: 0.24E+01 at ( 25, 30, 22)
       Min divergence: -.39E+01 at ( 26, 18, 31)
       Number of Sprinkler Droplets:        615
       Total Heat Release Rate:         7560.777 kW
       Radiation Loss to Boundaries:    6776.244 kW
       Mesh  2, Cycle   2914
       CPU/step:     1.887 s, Total CPU:      1.53 hr
       Time step:  0.03045 s, Total time:   128.87 s
       Max CFL number: 0.96E+00 at ( 21, 29, 42)
       Max divergence: 0.20E+01 at ( 22, 20, 22)
       Min divergence: -.60E+01 at (  7, 26, 48)
       Number of Sprinkler Droplets:        301

                         .
                         .
```

The Iteration number indicates how many time steps the code has run, whereas the Cycle number for a given mesh indicates how many time steps have been taken on that mesh. The date and time (wall clock time) are on the line starting with the word Iteration. The quantity `CPU/step` is the amount of CPU time required to complete a time step for that mesh; `Total CPU` is the amount of CPU time elapsed since the start of the run; `Time step` is the time step size for the given mesh; `Total time` is the time of the simulation;

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`Max/Min divergence` is the max/min value of the function $\nabla \cdot \mathbf{u}$ and is used as a diagnostic when the flow is incompressible (*i.e.* no heating); and `Max CFL number` is the maximum value of the CFL number. The `Radiation Loss to Boundaries` is the amount of energy that is being radiated to the boundaries. As compartments heat up, the energy lost to the boundaries can grow to be an appreciable fraction of the `Total Heat Release Rate`. Finally, `Number of Tracer Particles` indicates how many passive particles are being tracked at that time.

Following the completion of a successful run, a summary of the CPU usage per subroutine is listed. This is useful in determining where most of the computational effort is being placed.

19.2 Heat Release Rate and Related Quantities

The heat release rate of the fire, plus other global energy-related quantities, are automatically written into a text file called **CHID_hrr.csv**. The format of the file is as follows

```
s,kW,kW,kW,kW,kg/s,atm,atm
FDS_HRR_Time,HRR,RAD_LOSS,CONV_LOSS,COND_LOSS,BURN_RATE,ZONE_01,ZONE_02, ...
 0.0000000E+000, 0.0000000E+000, ...
 3.5355338E-001, 0.0000000E+000, ...
 .
 .
 .
```

`HRR` is the total heat release rate, `RAD_LOSS` is the amount of thermal radiation lost to the boundaries, `CONV_LOSS` is the rate of energy that is flowing out of (positive) or into (negative) the computational domain, `COND_LOSS` is the rate of energy that is being conducted into (positive) or out of (negative) the solid surfaces, `BURN_RATE` is the total mass loss rate of fuel, and `ZONE_01`, *etc.*, are the background pressures of the various pressure `ZONE`s.

Details of the integrated energy quantities can be found in Section 14.3.1. The background pressure is discussed in Section 9.6.

19.3 Device Output Data

Data associated with particular devices (link temperatures, smoke obscuration, thermocouples, etc.) specified in the input file under the namelist group `DEVC` is output in comma delimited format in a file called **CHID_devc.csv**. The format of the file is as follows

```
s        , UNITS(1) , UNITS(2) , ... , UNITS(N_DEVC)
FDS Time , ID(1)    , ID(2)    , ... , ID(N_DEVC)
T(1)     , VAL(1,1) , VAL(2,1) , ... , VAL(N_DEVC,1)
T(2)     , VAL(1,2) , VAL(2,2) , ... , VAL(N_DEVC,2)
                       .
                       .
                       .
```

where `N_DEVC` is the number of devices, `ID(I)` is the user-defined ID of the `I`th device, `UNITS(I)` the units, `T(J)` the time of the `J`th dump, and `VAL(I,J)` the value at the `I`th device at the `J`th time. The files can be imported into Microsoft Excel or almost any other spread sheet program. If the number of columns exceeds 256, the file will automatically be split into smaller files.

19.4 Control Output Data

Data associated with particular control functions specified in the input file under the namelist group `CTRL` is output in comma delimited format in a file called **CHID_ctrl.csv**. The format of the file is as follows

```
s,status,status,status,status
FDS Time,ID(1),ID(2),...,ID(N_CTRL)
 0.00000E+000,-001, 001, ...
 1.11803E-001,-001,-001, ...
             .
             .
             .
```

where `N_CTRL` is the number of controllers, `ID(I)` is the user-defined ID of the `I`th control function, and plus or minus 1's represent the state `-1 = .FALSE.` and `+1 = .TRUE.` of the `I`th control function at the particular time. The files can be imported into Microsoft Excel or almost any other spread sheet program. If the number of columns exceeds 256, the file will automatically be split into smaller files.

19.5 Gas Mass Data

The total mass of the various gas species at any instant in time is reported in the comma delimited file **CHID_mass.csv**. The file consists of several columns, the first column containing the time in seconds, the second contains the total mass of all the gas species in the computational domain in units of kg, the next lines contain the total mass of the individual species.

You must specifically ask that this file be generated, as it can potentially cost a fair amount of CPU time to generate. Set `MASS_FILE=.TRUE.` on the `DUMP` line to create this output file.

19.6 Mixture Fraction State Relations

The functional dependence of the mass fraction of the reactants and products of combustion on the mixture fraction is reported in the comma delimited file **CHID_state.csv**. The file consists of nominally 10 columns, the first column containing the mixture fraction, the last column the average molecular weight, and the rest the mass fractions of the various gas species in the case where complete combustion has occurred.

You must specifically ask that this file be generated. Set `STATE_FILE=.TRUE.` on the `DUMP` line to create this output file. If you forget to do this, you can easily re-run the case (remember to rename it something else!) for a few time steps. This file is created before the time iterations even begin.

19.7 Slice Files

The slice files defined under the namelist group `SLCF` are named **CHID_n.sf** (*n*=01,02...), and are written out unformatted, unless otherwise directed. These files are written out from **dump.f** with the following lines:

```
WRITE(LUSF) QUANTITY
WRITE(LUSF) SHORT_NAME
WRITE(LUSF) UNITS
WRITE(LUSF) I1,I2,J1,J2,K1,K2
WRITE(LUSF) TIME
WRITE(LUSF) (((QQ(I,J,K),I=I1,I2),J=J1,J2),K=K1,K2)
```

```
             .
             .
             .
      WRITE(LUSF) TIME
      WRITE(LUSF) (((QQ(I,J,K),I=I1,I2),J=J1,J2),K=K1,K2)
```

QUANTITY, SHORT_NAME and UNITS are character strings of length 30. The sextuplet (I1,I2,J1,J2,K1,K2) denotes the bounding mesh cell nodes. The sextuplet indices correspond to mesh cell nodes, or corners, thus the entire mesh would be represented by the sextuplet (0,IBAR,0,JBAR,0,KBAR).

There is a short Fortran 90 program provided, called **fds2ascii.f**, that can convert slice files into text files that can be read into a variety of graphics packages. The program combines multiple slice files corresponding to the same "slice" of the computational domain, time-averages the data, and writes the values into one file, consisting of a line of numbers for each node. Each line contains the physical coordinates of the node, and the time-averaged quantities corresponding to that node. In particular, the graphics package Tecplot reads this file and produces contour, streamline and/or vector plots. See Section 14.4 for more details about the program **fds2ascii**.

19.8 Plot3D Data

Quantities over the entire mesh can be output in a format used by the graphics package **Plot3D**. The Plot3D data sets are single precision (32 bit reals), whole and unformatted. Note that there is blanking, that is, blocked out data points are not plotted. If the statement WRITE_XYZ=.TRUE. is included on the DUMP line, then the mesh data is written out to a file called **CHID.xyz**

```
      WRITE(LU13)  IBAR+1,JBAR+1,KBAR+1
      WRITE(LU13)  (((X(I),I=0,IBAR),J=0,JBAR),K=0,KBAR),
      .            (((Y(J),I=0,IBAR),J=0,JBAR),K=0,KBAR),
      .            (((Z(K),I=0,IBAR),J=0,JBAR),K=0,KBAR),
      .        (((IBLK(I,J,K),I=0,IBAR),J=0,JBAR),K=0,KBAR)
```

where X, Y and Z are the coordinates of the cell corners, and IBLK is an indicator of whether or not the cell is blocked. If the point (X,Y,Z) is completely embedded within a solid region, then IBLK is 0. Otherwise, IBLK is 1. Normally, the mesh file is not dumped.

The flow variables are written to a file called **CHID_****_**.q**, where the stars indicate a time at which the data is output. The file is written with the lines

```
      WRITE(LU14)  IBAR+1,JBAR+1,KBAR+1
      WRITE(LU14)  ZERO,ZERO,ZERO,ZERO
      WRITE(LU14)  ((((QQ(I,J,K,N),I=0,IBAR),J=0,JBAR),K=0,KBAR),N=1,5)
```

The five channels N=1,5 are by default the temperature (°C), the u, v and w components of the velocity (m/s), and the heat release rate per unit volume (kW/m^3). Alternate variables can be specified with the input parameter PLOT3D_QUANTITY(1:5) on the DUMP line. Note that the data is interpolated at cell corners, thus the dimensions of the Plot3D data sets are one larger than the dimensions of the computational mesh.

Smokeview can display the Plot3D data. In addition, the Plot3D data sets can be read into some other graphics programs that accept the data format. This particular format is very convenient, and recognized by a number of graphics packages, including AVS, IRIS Explorer and Tecplot [1].

---

[1] With the exception of Smokeview, the graphics packages referred to in this document are not included with the source code, but are commercially available.

19.9 Boundary Files

The boundary files defined under the namelist group `BNDF` are named **CHID_*n*.bf** (*n*=0001,0002...), and are written out unformatted. These files are written out from **dump.f** with the following lines:

```
WRITE(LUBF) QUANTITY
WRITE(LUBF) SHORT_NAME
WRITE(LUBF) UNITS
WRITE(LUBF) NPATCH
WRITE(LUBF) I1,I2,J1,J2,K1,K2,IOR,NB,NM
WRITE(LUBF) I1,I2,J1,J2,K1,K2,IOR,NB,NM
             .
             .
             .
WRITE(LUBF) TIME
WRITE(LUBF) (((QQ(I,J,K),I=11,I2),J=J1,J2),K=K1,K2)
WRITE(LUBF) (((QQ(I,J,K),I=11,I2),J=J1,J2),K=K1,K2)
             .
             .
             .
WRITE(LUBF) TIME
WRITE(LUBF) (((QQ(I,J,K),I=11,I2),J=J1,J2),K=K1,K2)
WRITE(LUBF) (((QQ(I,J,K),I=11,I2),J=J1,J2),K=K1,K2)
             .
             .
             .
```

`QUANTITY`, `SHORT_NAME` and `UNITS` are character strings of lengths 60, 30 and 30, respectively. `NPATCH` is the number of planes (or "patches") that make up the solid boundaries plus the external walls. The sextuplet (`I1,I2,J1,J2,K1,K2`) defines the cell nodes of each patch. `IOR` is an integer indicating the orientation of the patch ($\pm 1, \pm 2, \pm 3$). You do not prescribe these. `NB` is the number of the boundary (zero for external walls) and `NM` is the number of the mesh. Note that the data is planar, thus one pair of cell nodes is the same. Presently, Smokeview is the only program available to view the boundary files.

19.10 Particle Data

Coordinates and specified quantities related to tracer particles, sprinkler droplets, and other Lagrangian particles are written to a FORTRAN unformatted (binary) file called **CHID.prt5**. Note that the format of this file has changed from previous versions (4 and below). The file consists of some header material, followed by particle data output every `DT_PART` seconds. The time increment `DT_PART` is specified on the `DUMP` line. It is `T_END/NFRAMES` by default. The header materials is written by the following FORTRAN code in the file called **dump.f90**.

```
WRITE(LUPF) ONE_INTEGER            ! Integer 1 to check Endian-ness
WRITE(LUPF) NINT(VERSION*100.)     ! FDS version number
WRITE(LUPF) N_PART                 ! Number of PARTicle classes
DO N=1,N_PART
   PC => PARTICLE_CLASS(N)
   WRITE(LUPF) PC%N_QUANTITIES,ZERO_INTEGER  ! ZERO_INTEGER is a place holder
   DO NN=1,PC%N_QUANTITIES
      WRITE(LUPF) CDATA(PC%QUANTITIES_INDEX(NN))  ! 30 character output quantity
      WRITE(LUPF) UDATA(PC%QUANTITIES_INDEX(NN))  ! 30 character output units
   ENDDO
ENDDO
```

Note that the initial printout of the number 1 is used by Smokeview to determine the Endian-ness of the file. The Endian-ness has to do with the particular way real numbers are written into a binary file. The version number is used to distinguish new versus old file formats. The parameter N_PART is not the number of particles, but rather the number of particle classes corresponding to the PART namelist groups in the input file. Every DT_PART seconds the coordinates of the particles and droplets are output as 4 byte reals:

```
WRITE(LUPF) REAL(T,FB)  ! Write out the time T as a 4 byte real
DO N=1,N_PART
   WRITE(LUPF) NPLIM    ! Number of particles in the PART class
   WRITE(LUPF) (XP(I),I=1,NPLIM),(YP(I),I=1,NPLIM),(ZP(I),I=1,NPLIM)
   WRITE(LUPF) (TA(I),I=1,NPLIM)  ! Integer "tag" for each particle
   IF (PC%N_QUANTITIES > 0) WRITE(LUPF) ((QP(I,NN),I=1,NPLIM),NN=1,PC%N_QUANTITIES)
ENDDO
```

The particle "tag" is used by Smokeview to keep track of individual particles and droplets for the purpose of drawing streamlines. It is also useful when parsing the file. The quantity data, QP(I,NN), is used by Smokeview to color the particles and droplets. Note that it is now possible with the new format to color the particles and droplets with several different quantities.

19.11 Profile Files

The profile files defined under the namelist group PROF are named **CHID_prof_*nn*.csv** (*nn*=01,02...), and are written out formatted. These files are written out from **dump.f** with the following line:

```
WRITE(LU_PROF) T,NWP+1,(X_S(I),I=0,NWP),(Q(I),I=0,NWP)
```

After the time T, the number of node points is given and then the node coordinates. These are written out at every time step because the wall thickness and the local solid phase mesh may change over time due to the solid phase reactions. Array Q contains the values of the output quantity, which may be wall temperature, density or component density.

19.12 3-D Smoke File Format

3-D smoke files contain alpha values used by Smokeview to draw semi-transparent planes representing smoke and fire. FDS outputs 3-D smoke data at fixed time intervals, but unlike other output data, the file format is C, not Fortran. Note that char's are one byte, and "int's" and float's are four bytes. A *pseudo-code* representation of the 3-D smoke file is given by:

```
endian flag (int)
is1, is2, js1, js2, ks1, ks2 (6*int)
version (int)
for each time:
   time  (float)
   chars_uncompressed, chars_compressed (2*int)
   compressed_data (chars_compressed*char)
end time
```

The endian flag is an integer one. Smokeview uses this number to determine whether the computer creating the 3-D smoke file and the computer viewing the 3-D smoke file use the same or different byte swap (endian) conventions for storing floating point numbers. The opacity data is compressed using run-length encoding (RLE).

19.13 Isosurface File Format

Iso-surface files are used to store one or more surfaces where the specified QUANTITY is a specified value. FDS outputs iso-surface data at fixed time intervals. As with 3-D smoke, the file format is C, not Fortran. Note that char's are one byte, short's are two bytes and "int's" and float's are four bytes. A *pseudo-code* representation of the iso-surface file is given by:

```
version                              (int)
len1,len2,len3                       (3*int)
label1,label2,label3                 ((len1+len2+len3+4)*char)
nlevels                              (int)
level_1, level_2, ..., level_nlevels (nlevels*float)
for each time:
  time                               (float)
  for each level
    nvertices                        (int)
    ntriangles                       (int)
    vertices_1, ..., vertex_nvertices  (3*short*nvertices)
    triangles_1, ..., triangle_ntriangles (3*(byte/short/float)*ntriangles)
  end level
end time
```

The length of each triangles_i node is one byte if the number of triangles, ntriangles, is between zero and 255 (inclusive), two bytes if ntriangles is between 256 and 65536 (inclusive) and four bytes if ntriangles is greater than or equal to 65536.

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