## NIST GCR 11-955

# Multi-Parameter, Multiple Fuel Mixture Fraction Combustion Model for Fire Dynamics Simulator



## **NIST GCR 11-955**

# Multi-Parameter, Multiple Fuel Mixture Fraction Combustion Model for Fire Dynamics Simulator

Jason Floyd Hughes Associates, Inc. Fire Science & Engineering 3610 Commerce Dr., Suite 817 Baltimore, MD 21227

Grant 70NANB8H8161

December 2011



U.S. Department of Commerce John E. Bryson, Secretary

National Institute of Standards and Technology Patrick D. Gallagher, Under Secretary of Commerce for Standards and Technology and Director Notice

This report was prepared for the Engineering Laboratory of the National Institute of Standards and Technology under Grant number 70NANB8H8161. The statement and conclusions contained in this report are those of the authors and do not necessarily reflect the views of the National Institute of Standards and Technology or the Engineering Laboratory.

## Multi-Parameter, Multiple Fuel Mixture Fraction Combustion Model for Fire Dynamics Simulator

Final Progress Report Reporting Period September 1, 2008 through August 31, 2011

Grant # 70NANB8H8161

Submitted on November 9, 2011

Prepared for Dr. Kevin McGrattan Engineered Fire Safety Group



**National Institute of Standards and Technology** Technology Administration, U.S. Department of Commerce

> 100 Bureau Dr, Stop 8663 Gaithersburg, MD 20899

> > Prepared by Dr. Jason Floyd Senior Researcher



3610 Commerce Dr., #817 Baltimore, MD 21227 Tel: (410) 767-8677 Fax: (410) 767-8688

## TABLE OF CONTENTS

1.0	Sumn	nary of Work Performed During Annual Reporting Period	. 1
1.1	Ma	jor Accomplishments	1
1.2		nor Accomplishments	
2.0		cations	
3.0		Documentation	
4.0	Major	FDS Enhancements	3
4.1		cies Tracking	
4.2		w Combustion Framework	
4.3		AC Network Model	
	.3.1	Boundary Conditions of the HVAC Solver	
4	.3.2	Boundary Conditions of the CFD Solver	
4	.3.3	Leakage Flows	11
4	.3.4	Filtration	
4	.3.5	Heating/Cooling	
4.4	Dep	position	13
5.0	Minor	r Enhancements	14
5.1	Dro	pplet Evaporation	14
5.2	Ent	halpy Diffusion	16
5.3	The	ermophysical Properties	16
5.4	Spe	cies Database	16
5.5	Inp	ut File Readability Improvements	18
5	.5.1	Relocated Inputs	18
5	.5.2	Input Consistency	18
5	.5.3	Defining Reactions	19
5.6	Nev	w Output Quantities	20
5.7	&R	AMP DEVC_ID	21
5.8	&S	URF NET_HEAT_FLUX	21
5.9	Ter	nperature Dependent Species Properties	21
6.0		Support	
		A: FDS Releases	
APPE	NDIX	B: Source Code Commits to GoogleCode	23
		C: Issues Addressed	
APPE	NDIX	D: Discussion Forum	14

## 1.0 Summary of Work Performed During Annual Reporting Period

This report summarizes FDS development and support activities performed during the three year grant period of 70NANB8H8161. A brief overview of the major and minor accomplishments are provided below. More detailed discussions follow in the remainder of this report.

1.1 Major Accomplishments

Major accomplishments during the grant include:

- Implementing a new scheme for tracking species
- Implementing a new framework for combustion modeling
- Adding an HVAC network model
- Adding soot deposition capabilities
- Release of 3 minor and 12 maintenance versions of FDS (a summary is Appendix A)
- 1.2 Minor Accomplishments

Some of the notable minor accomplishments include

- Improvements to droplet evaporation
- Improvements to the computation of thermal physical properties
- Extended database of gaseous and liquid properties
- Readability improvements to the input file
- Reorganization of inputs

The appendices to this report contain a summary of FDS releases (Appendix A), a summary of all commits to the FDS repository (Appendix B), a summary of all Issue Tracker issues responded to by the author (Appendix C), and a summary of all research publications produced by the author (below).

#### 2.0 Publications

Floyd, J. and McGrattan, K., "Extending the Mixture Fraction Concept to Address Under Ventilated Fires," *Fire Safety Journal*, **44** (3): 291–300.

J. Floyd and K. McGrattan. Validation of a CFD Fire Model Using Two-Step Combustion Chemistry Using the NIST Reduced Scale Ventilation-Limited Compartment Data. *Fire Safety Science* **9**:117-128.

D. Gottuk, C. Mealy, and J. Floyd. Smoke Transport and FDS Validation. *Fire Safety Science* **9**:129-140.

J. Floyd. Coupling a Network HVAC Model to a Computation Fluid Dynamics Model Using Large Eddy Simulation. In 12th International Conference on Fire Science and Engineering: Interflam, University of Nottingham, UK, July 5-7, 2010.

J. Floyd and R. McDermott. Modeling Soot Deposition Using Large Eddy Simulation with a Mixture Fraction Based Framework. In 12th International Conference on Fire Science and Engineering: Interflam, University of Nottingham, UK, July 5-7, 2010.

K. McGrattan, R. McDermott, W. E. Mell, G. Forney, J. Floyd, S. Hostikka, and A. Matala. Modeling the Burning of Complicated Objects Using Lagrangian Particles. In 12th International Conference on Fire Science and Engineering: Interflam, University of Nottingham, UK, July 5-7, 2010.

J. Williamson, C. Beyler, and J. Floyd. Validation of Numerical Simulations of Compartments with Forced or Natural Ventilation Using the Fire and Smoke Simulator (FSSIM), CFAST, and FDS. In 12th International Conference on Fire Science and Engineering: Interflam, University of Nottingham, UK, July 5-7, 2010.

Boehmer, H.R., Floyd, J.E., and Gottuk, D.T., "Evaluation of Calorimeter Heat Release Rate as Input to FDS Model for Simulation of Underventilated Compartment Fires," Proceedings – 2010 International Symposium on Fire Investigation Science and Technology, University of Maryland University College, September 28–29, 2010, pp. 93–104.

Hofmeister, C. et al., *SFPE Engineering Guide: Guidelines for Substantiating a Fire Model for a Given Application*, SFPE G.06 2011, Society of Fire Protection Engineers, Bethesda, MD, 2011.

J. Floyd. Coupling a Network HVAC Model to a Computation Fluid Dynamics Model Using Large Eddy Simulation. In 10th International Symposium, IAFSS, University of Maryland, June 19-24, 2011

R. McDermott, K. McGrattan, and J. Floyd. A Simple Reaction Time Scale for Under-Resolved Fire Dynamics. In 10th International Symposium, IAFSS, University of Maryland, June 19-24, 2011.

J. Vaari, J. Floyd, and R. McDermott. CFD Simulations of Co-Flow Diffusion Flames. In 10th International Symposium, IAFSS, University of Maryland, June 19-24, 2011.

J. Williamson, C. Beyler, and J. Floyd. Validation of Numerical Simulations of Compartments with Forced or Natural Ventilation Using the Fire and Smoke Simulator (FSSIM), CFAST, and FDS. In 10th International Symposium, IAFSS, University of Maryland, June 19-24, 2011.

J. Floyd. Coupling a Network HVAC Model to a Computation Fluid Dynamics Model Using Large Eddy Simulation. In Proceedings, Fire and Evacuation Modeling Technical Conference, Baltimore, MD, August 15-16, 2011

## **3.0 FDS Documentation**

As part of continued efforts to improve software quality assurance for FDS, a Configuration Management Plan was created and added to the repository. The configuration management plan defines the roles and responsibilities of the development team members, the process for maintaining configuration control and the items that are under control, the process for handling change requests (bug reports and user requests for enhancement), and the process for issuing new versions.

## 4.0 Major FDS Enhancements

A full listing of FDS code changes during this reporting period is provided in Appendix B.

4.1 Species Tracking

FDS v5 had two approaches to tracking species. The user could define all species individually (referred to as primitive species), or the user could make use of a lumped species approach to track fuel, air, and combustion products. The lumped species reduced the computational burden by reducing the number of transport equations being solved by FDS. The lumped species implementation was very limited, however, in that user had little control over the specification of the lumped species and that its use was limited to the mixing controlled combustion model within FDS. In addition to the limitations in reaction scheme, the lumped species were limited to fuel chemistries of C, H, O, and N with products of soot, CO<sub>2</sub>, H<sub>2</sub>O, CO, N<sub>2</sub>, and H<sub>2</sub>. Users wanting to track other species, such as HCl, had no easy way of doing so.

The solution was to treat all species as lumped species and provide the user with the ability to customize the lumped species definitions. Changes to the combustion model, Section 4.2, were made to use the lumped species definitions and hence enable the use of primitive or lumped species in any of the reaction schemes (i.e. either Arrhenius rate or mixing controlled).

FDS v6 will have three methods of defining the species being used in FDS:

- 1. A simple chemistry option which will replicate the previous lumped species approach (e.g. fuels containing only C, H, O, and N). For the majority of FDS user this will be the method used and there will be little change to the input file format from that of FDS v5.
- 2. An option to specify all species as primitive species. This input option will also remain essentially identical to FDS v5 with the exception that there will be more flexibility for specifying species reactions.
- 3. An option to define custom lumped species. This will allow users to define reactions that produce species other than soot, CO<sub>2</sub>, H<sub>2</sub>O, CO, N<sub>2</sub>, and H<sub>2</sub> and still, for example, be able to track products as a single species.

Implementing this approach required a few sets of changes to FDS v5. First the inputs for species (&SPEC input group) required modification. The keyword SMIX\_COMPONENT\_ONLY was added to the namelist group. This keyword denotes that the species being defined is not to be tracked as a primitive species, but only as part of a lumped species (i.e. FDS will not solve a

separate transport equation for that species). Second a new input group was created for defining custom lumped species. This new input group is called &SMIX and it has the following variables available to it:

BACKGROUND	Denotes the lumped species is to be used as the background
Difference	species
ID	Name of the lumped species
MASS_FRACTION	Mass fractions of the subspecies making up the lumped species
MASS_PRACTION	(define one of MASS_FRACTION or VOLUME_FRACTION)
MASS_FRACTION_0	Initial mass fraction of the lumped species
SPEC ID	Names of the subspecies making up the lumped species (must
SFEC_ID	match an ID from a &SPEC input)
VOLUME FRACTION	Mass fractions of the subspecies making up the lumped species
VOLUME_PRACTION	(define one of MASS_FRACTION or VOLUME_FRACTION)

An example of the three methods of defining species is shown below. Each example represents the species required for the complete combustion of propane with no soot or CO yield and with the assumption that the ambient air consists of only  $N_2$  and  $O_2$ . Below are the required &SPEC, &SMIX, and &REAC inputs (the details of the &REAC input changes will be discussed in Section 4.2):

1. Using Simple Chemistry Inputs:

```
&REAC FUEL='PROPANE', SOOT_YIELD=0.0,Y_CO2_INFTY=0.0,
HUMIDITY=0.0, Y_O2_INFTY=0.23 /
```

With this set of inputs FDS will automatically create lumped species called AIR (the background species), PROPANE and PRODUCTS. There will be two species transport equations (PROPANE and PRODUCTS), and the lumped BACKGROUND species (AIR) is inferred by conservation of mass.

2. Using Primitive Species Inputs:

```
&SPEC ID='NITROGEN', BACKGROUND=.TRUE./
&SPEC ID='OXYGEN', MASS_FRACTION_0=0.23/
&SPEC ID='PROPANE'/
&SPEC ID='WATER VAPOR', MASS_FRACTION_0=0.0/
&SPEC ID='CARBON DIOXIDE'/
&REAC FUEL='PROPANE', EQUATION='PROPANE+5*02=3*C02+4*H20',
HEAT_OF_COMBUSTION=47531.282 /
```

With this set of inputs FDS will automatically create lumped species (although each will only have the one sub-species) for each of the primitive species. In this implementation there will be four species transport equations (OXYGEN, PROPANE, WATER VAPOR, CARBON DIOXIDE), and the BACKGROUND species (NITROGEN) is inferred by conservation of mass.

3. Using Custom Lumped Species Inputs:

```
&SPEC ID='NITROGEN', SMIX_COMPONENT_ONLY=.TRUE./
&SPEC ID='OXYGEN', SMIX_COMPONENT_ONLY=.TRUE./
&SPEC ID='WATER VAPOR', SMIX_COMPONENT_ONLY=.TRUE./
&SPEC ID='CARBON DIOXIDE', SMIX_COMPONENT_ONLY=.TRUE./
&SMIX ID='AIR',
SPEC_ID='NITROGEN', 'OXYGEN', MASS_FRACTION=0.77,0.23,
BACKGROUND=.TRUE./
&SMIX ID='PRODUCTS', SPEC_ID='NITROGEN', 'WATER VAPOR', 'CARBON
DIOXIDE', MASS_FRACTION=0.72409946,0.09741653,0.17848401/
&REAC FUEL='PROPANE',
EQUATION='PROPANE+24.12056683*AIR=26.12056683*PRODUCTS',
HEAT_OF_COMBUSTION=47531.282 /
```

With this set of inputs there will be two species transport equations (PROPANE and PRODUCTS), and the lumped BACKGROUND species (AIR) is inferred by conservation of mass.

Within the FDS documentation the variable  $Y_i$  will be used to represent the i<sup>th</sup> primitive species and the variable  $Z_i$  will be used to represent the i<sup>th</sup> lumped species. A primitive species that is being tracked as a primitive species will be considered a lumped species by FDS (a lumped species with only one sub-species). To go from the lumped species to the primitive species, a matrix multiplication is performed. Using the example case above:

```
 \begin{aligned} A\vec{Z} &= \vec{Y} \\ \begin{vmatrix} 0.77 & 0.00 & 0.72 \\ 0.23 & 0.00 & 0.00 \\ 0.00 & 1.00 & 0.00 \\ 0.00 & 0.00 & 0.18 \\ 0.00 & 0.00 & 0.10 \end{vmatrix} \begin{vmatrix} Z_{Air} \\ Z_{Fuel} \\ Z_{Products} \end{vmatrix} = |Y_{N_2} \quad Y_{O_2} \quad Y_{C_3H_8} \quad Y_{CO_2} \quad Y_{H_2O}| \end{aligned}
```

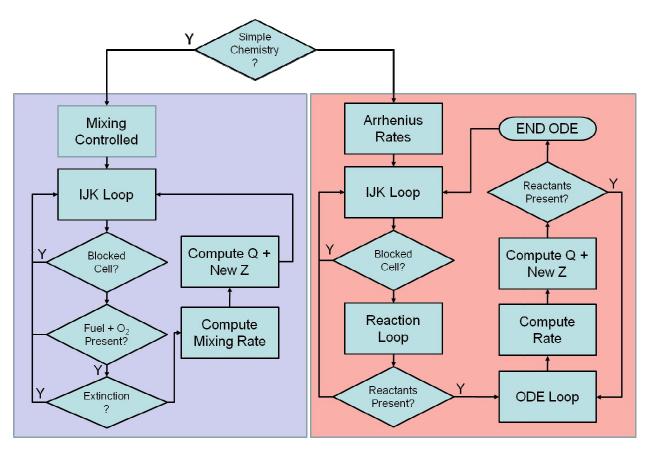
Thermophysical properties are evaluated in a similar manner. For example the specific heat of the gas in the grid cell *IJK* will be computed as

$$c_{p,IJK} = \sum_{i=1,nspecies} c_{p,i}(T_{IJK})Y_i = \overrightarrow{c_p}(T_{IJK}) \cdot \overrightarrow{Y} = \overrightarrow{c_p}(T_{IJK}) \cdot A\overrightarrow{Z} = \overrightarrow{c_{p,Z}}(T_{IJK}) \cdot \overrightarrow{Z}$$

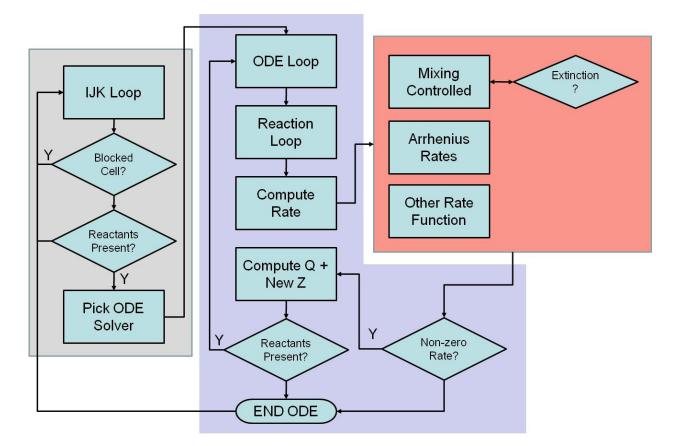
Similar functions can be used for conductivity, viscosity, and the average molecular weight. Additional details on changes to thermophysical properties in FDS can be found in Section 5.2.

#### 4.2 New Combustion Framework

As briefly mentioned in the previous section, FDS v5 had two combustion models. A finite-rate model which could be used only with primitive species and a mixing controlled model which could only be used if simple chemistry inputs were provided. These models were handled by two entirely separate routines. This is depicted in the figure below.



From the viewpoint of code maintainability, user flexibility, and future development, this balkanization made little sense. From a mathematical viewpoint there is little difference between the two combustion approaches. In the finite rate model, a reaction rate is determined using the Arrhenius expression and then an ODE for the species is solved. In the mixing controlled model, a reaction rate is determined from a mixing time and then an ODE for the species is solved. The difference between the two approaches is the rate computation. Maintaining two blocks of code that essentially replicate each other adds needless complexity to the source code and makes it harder for new reaction schemes to be developed and tested. Instead the combustion routine was reorganized as shown:



In this approach one subroutine handles the global loop over the geometry and if a reaction is possible (i.e. all reactants are present) it calls an ODE solver (that is user selectable). This solver is passed nothing more than a vector of the species that are present and the grid cell location and it returns an updated species vector and a heat release rate. Within each ODE solver a reaction rate must be determined for each chemical reaction. This is done by a call to reaction rate top level routine. This routine is passed the current species vector and the grid cell location. Based on the individual reaction inputs, a rate function is selected and evaluated.

In FDS v5, the reaction rate type and the ODE solver was dictated by how species inputs were provided. In the new scheme the ODE solver becomes user selectable and adding new ODE solvers is trivial as there is a well defined calling sequence for the solver. A user merely needs to code the solver to accept the standard calling data and add the solver name to the list of available solvers. No additional coding is needed to compute reaction rates or do the global loop over the geometry. Similarly, in the new scheme, each reaction can be provided with its own rate type (i.e. users could mix Arrhenius rates with mixing controlled rates). A user could also easily add new reaction rate types to the source code without having to code the ODE solver or the global loop over the geometry. It is hoped that this generalized combustion solver will make it easier to develop and test new combustion approaches within FDS.

## 4.3 HVAC Network Model

The overall HVAC solver is based on the MELCOR (Gauntt, 2000) thermal hydraulic solver. MELCOR is a computer code for simulating accidents in nuclear power plant containment

buildings. The Fire and Smoke Simulator (FSSIM) (Floyd, 2003), a network fire model, has shown prior success in using the MELCOR solver to model fire spread and smoke movement in the presence of complex ventilation systems.

The MELCOR solver uses an explicit conservation of mass and energy combined with an implicit solver for the conservation of momentum. An HVAC system is represented as network of nodes and ducts where a node represents where a duct joins with the FDS computational domain or where multiple ducts are joined such as a tee. A duct segment in the network represents any continuous flow path not interrupted by a node and as such may include multiple fittings (elbows, expansions, contractions, etc.) and may have varying area over its length. The current implementation of the model does not account for mass storage within an HVAC network. The conservation equations are:

Mass:

$$\sum_{j \text{ connected to } i} \rho_j u_j A_j = 0,$$

Energy:

$$\sum_{j \text{ connected to } i} \rho_j u_j A_j h_j = 0, \text{ and }$$

Momentum:

$$\rho_j L_j \frac{du_j}{dt} = (P_i - P_k) + (\rho g \Delta z)_j + \Delta P_j$$
$$-\frac{1}{2} K_j \rho_j |u_j| u_j$$

Since nodes have no volume, the mass and energy conservation equations are merely what flows into a node, must also flow out of the node. In the momentum equation the terms on the right hand side are: the pressure gradient between the upstream and the downstream node, the buoyancy head, pressure rise due to an external source (e.g. a fan or blower), and the pressure losses due to wall friction or the presence of duct fittings. The momentum equation is discretized in time which yields:

$$u_{j}^{n} = u_{j}^{n+1} \frac{\Delta t^{n}}{\rho_{j} L_{j}} \left( \left( \tilde{P}_{i}^{n} - \tilde{P}_{k}^{n} \right) + \left( \rho g \Delta z \right)_{j}^{n-1} + \Delta P_{j}^{n-} \right) \\ - \frac{\Delta t^{n} K_{j}}{2L_{j}} \left( u_{j}^{n-} - u_{j}^{n+} | u_{j}^{n} - | u_{j}^{n+} | u_{j}^{n-} \right)$$

Note that the node pressures are not expressed as  $P_i^n$ , but rather as  $\tilde{P}_i^n$ . This indicates an extrapolated pressure at the end of the current time step rather than the actual pressure. The pressure in a compartment is a function of the mass and energy flows into and out of that compartment. If that compartment is connected to other compartments by doors or other openings, then the pressure is also dependent upon flows into and out those other compartments.

The mass and energy flows include both those being predicted by the HVAC model and those being predicted by the CFD model. Since the two models are not fully coupled, the extrapolated pressure is an estimate of the pressure at the end of the time step based upon the pressure rise for the prior time-step.

FDS decouples the pressure into a series of zone background pressures which vary with height but are otherwise constant in a pressure zone (a pressure zone is a region of the domain without a direct flow opening to another region such as a room with a closed door) and a dynamic pressure. The background pressure can change as a function of the mass and energy flows into or out of a pressure zone and is computed by summing the divergence inside of a pressure zone with the volume flows in and out of that pressure zone:

$$\frac{dP_m}{dt} = \left( \int_{\Omega_m} \mathsf{D}dV - \int_{d\Omega_m} \mathsf{u} \cdot dS \right) / \int_{\Omega_m} \mathsf{P}dV$$

We can therefore estimate the extrapolated pressure at the next time step as:

,

$$\widetilde{P}_m^n = P_m^{n-1} + \frac{dP_m^{n-1}}{dt} \Delta t^n$$

By removing the contribution of the prior time-step's HVAC contribution to the pressure rise, the extrapolated pressure can be expressed in terms of the HVAC solution for the current time step:

$$\widetilde{P}_{m}^{n} = P_{m}^{n-1} + \frac{dP_{m}^{n-1}}{dt} + \left( \sum_{j \text{ in } m} u_{j}^{n-1} A_{j}^{n-1} - \sum_{j \text{ in } m} u_{j}^{n} A_{j}^{n} \right) / \int_{\Omega_{m}} P dV = \widetilde{P}_{m,non-hvac}^{n} - \sum_{j \text{ in } m} u_{j}^{n} A_{j}^{n} / \int_{\Omega_{m}} P dV$$

Substituting into the velocity equation above:

$$\begin{split} u_{j}^{n} &\left(1 + \frac{K_{j}}{2L_{j}} \left| u_{j}^{n-} - u_{j}^{n+} \right| \right) - \\ \frac{\Delta t^{n^{2}}}{\rho_{j}L_{j}} &\left(\sum_{j \text{ in } i} u_{j}^{n} A_{j}^{n} \middle/ \int_{\Omega_{i}} P dV - \sum_{j \text{ in } k} u_{j}^{n} A_{j}^{n} \middle/ \int_{\Omega_{k}} P dV \right) \\ &= u_{j}^{n-1} + \\ \frac{\Delta t^{n}}{\rho_{j}L_{j}} &\left(\widetilde{P}_{i,non-hvac}^{n} - \widetilde{P}_{k,non-hvac}^{n} + (\rho g \Delta z)_{j}^{n-1} + \Delta P_{j}\right) \\ &+ \frac{K_{j}}{2L_{i}} \left| u_{j}^{n+} \right| u_{j}^{n-} \end{split}$$

The superscripts n + and n- on the velocity are used to linearize the flow loss in a duct to avoid a non-linear differential equation for velocity. The n + superscript is the prior iteration value and the n- is either the prior iteration value or zero if flow reversal occurred. This approach, rather than  $u_j^{n^2} \approx u_j^n u_j^{n-1}$ , is used to speed convergence when duct flows are near zero to avoid large changes in K if the forward and reverse losses are specified to be different.

In the previous equation, if either duct node is an internal node (i.e. it is not connected to the domain the CFD model is solving for), then extrapolated pressure terms are not included for that node and the node pressure is solved for directly. For example if node *i* were an internal node, the equation would become:

$$\begin{split} u_{j}^{n} \left(1 + \frac{K_{j}}{2L_{j}} \left| u_{j}^{n-} - u_{j}^{n+} \right| \right) - \\ \frac{\Delta t^{n}}{\rho_{j}L_{j}} \left( P_{i}^{n} + \Delta t^{n} \sum_{j \text{ in } k} u_{j}^{n} A_{j}^{n} / \int_{\Omega_{k}} P dV \right) \\ = u_{j}^{n-1} + \frac{\Delta t^{n}}{\rho_{j}L_{j}} \left( - \widetilde{P}_{k,non-hvac}^{n} + (\rho g \Delta z)_{j}^{n-1} + \Delta P_{j} \right) \\ + \frac{K_{j}}{2L_{i}} \left| u_{j}^{n+} \right| u_{j}^{n-} \end{split}$$

The above equation for each duct along with a mass conservation equation for each internal duct node results in a set of linear equations for duct velocities and node pressures. The set of equations is solved, and the solution checked for error in mass conservation, flow reversal in a duct, and the magnitude change of the duct velocity from the prior iteration (or time step if the first iteration). If any convergence check fails, the solution is re-iterated.

#### Multi-Parameter Combustion Model for FDS

#### 4.3.1 Boundary Conditions of the HVAC Solver

The HVAC solver requires boundary conditions of pressure, temperature, and species for each duct node coupled to the CFD domain. For flows from a duct to the CFD domain, temperature and species are those of the duct. For flows from the CFD domain to a duct, the temperature and species are taken as the density weighted average of the gas cells adjacent to the vent coupling the CFD domain to the HVAC domain. Pressure is taken as the area weighted total pressure (background pressure plus dynamic pressure) over the vent. The total pressure is used so that the HVAC solver properly accounts for the direct impingement of fire driven flows onto a vent.

#### 4.3.2 Boundary Conditions of the CFD Solver

The flows predicted by the HVAC solver are coupled to the CFD domain as vents of specified mass flux and temperature. The mass flux boundary condition is given by:

$$\dot{m}_{w,a}'' = Y_{j,a}u_jA_j\rho_j/A_{CFD VENT}$$

The wall temperature boundary condition is the duct temperature for flows into the CFD domain and the neighboring gas cell temperature for no flow or flows from the CFD domain. The boundary conditions for velocity, density, and species are given by:

$$\rho_{w} = \frac{\overline{W_{w}P}}{RT_{w}}; \quad \overline{W_{w}} = f(Y_{w})$$

$$Y_{w,a} = \frac{\dot{m}''_{w,a} + \frac{(\rho D)_{w}}{\Delta x_{w}} Y_{g,a}}{\frac{(\rho D)_{w}}{\Delta x_{w}} + u_{w}\rho_{w}}$$

$$u_{w} = \frac{\sum_{w} \dot{m}''_{w,a}}{\rho_{w}A_{w}}$$

These variables are all coupled to one another; therefore, the solution is iterated. In most cases the boundary values change slowly from time step to time step and thus little iteration is required.

#### 4.3.3 Leakage Flows

FDS v5 contained a simple, explicit solver for computing leakage flows between compartments. The model required the user to identify pressure zones, enclosed regions where the background pressure would rise or fall independent of other regions, using the keyword &ZONE. As part of the zone definition, the user could identify how much leakage area was present from one zone to another. That leakage area was then assigned to surfaces using the LEAK\_PATH input on the &SURF definition. This approach had three major issues associated with it:

1. It did not pass species through a leak. Therefore, toxic combustion products and soot would not leak from a fire compartment to an adjacent space.

- 2. The explicit solver meant that either large leakage areas or large numbers of leakage paths resulted in numerical instabilities due to over/undershooting the leakage flows over a time step. These instabilities often resulted in stopped FDS execution and/or unrealistic leakage flows and compartment pressures.
- 3. The existing solver could not be directly coupled to the HVAC solver.

A leak path, however, can be thought of as a special class of HVAC system. There is an inlet and an outlet node (a wall, a doorway, etc.) which are joined by a small area duct (the leakage path). Instead of the explicit leakage flow solver in FDS v5, FDS v6 will utilize the HVAC solver. Each user defined leakage path will be converted into an equivalent pair of duct nodes connected by a duct. Using the HVAC solver allows for the transport of species through leaks and eliminates the risk of numerical instabilities as the HVAC solver is implicit. One additional assumption was required to implement the new leakage solver. This assumption is that the leakage flows are small enough that the discharge temperature of the leak is at equilibrium with the wall temperature on the discharge side (e.g. the wall is acting as a perfect heat exchanger). That is the surface temperature of the leaking surface is based upon the normal surface temperature routines and not the temperature that results from the HVAC solution.

## 4.3.4 Filtration

HVAC systems commonly contain air filters for the removal of particulates. In many cases these filters are relatively coarse and primarily remove very large particulates or aggregations of particulates (to prevent damage to the blower). For some applications such as clean rooms, medical facilities, and facilities handling radioactive materials, the filters may be very fine (e.g. HEPA). Under fire conditions these filters can clog, preventing the flow of air, or if blowers are powerful enough, rupture and release their contents. The HVAC model has the ability to model the removal of particulate matter by a filter and to account for the increased flow resistance that results from the increased loading on the filter.

Filters are implemented as a special class of duct node. A filter is defined with an efficiency (the fraction of the mass of a species passing through the filter that is removed by the filter) and a flow loss vs. filter loading curve that defines how the flow loss through the filter increases with filter loading. The HVAC solver treats the species removal as a duct flow. A duct flow equation is created that removes the user defined fraction of mass of the species flowing through the filter. Filter nodes are limited to only having two ducts attached to the filter (an inlet and an outlet). This simplifies the duct equation for the filter loss as it simply becomes a multiplier of the upstream duct equation.

## 4.3.5 Heating/Cooling

In addition to filtrations, HVAC systems contain equipment for the heating and/or cooling of air. The HVAC model contains a simple heat exchanger model to account for the heating and cooling. An aircoil is defined as special class of duct that has either a fixed quantity of heat removal or addition or has a temperature and mass flow of a working fluid along with a heat exchanger effectiveness. In the later case the outlet temperature of the aircoil is computed by first determining the maximum possible temperature change (the temperature where heat exchange makes the aircoil working fluid and the gas exit temperatures equal). The total heat

exchange for that temperature difference is determined and multiplied by the efficiency. The new quantity of heat exchange is used to compute the exit temperature. The aircoil can be assigned a device or control function that will determine whether or not the aircoil is operating. For example a DEADBAND control function could be used to turn on a cooling coil when the temperature in a room rises above a setpoint and then turn off the coil when the temperature falls below the setpoint.

#### 4.4 Deposition

The International Collaborative Fire Model Project (ICFMP) Benchmark Series 3 tests included data on soot obscuration within the test compartment. All fire models predicted much larger levels of obscuration over the duration of the test than actually occurred with generally larger errors for closed door test than for the open door tests. A brief set of experiments performed during a FPRF project on smoke detectors suggested that the deposition of soot on surfaces may be a more significant phenomenon than previously thought. A simple soot deposition model was added to FDS that included both thermophoretic and turbulent deposition mechanisms. Thermophoretic deposition is modeled as:

$$u_{therm} = 2C_s \frac{\left(\frac{k_g}{k_s} + C_t K_n\right) \left(1 + K_n \left(A_1 + A_2 e^{-\frac{2A_3}{K_n}}\right)\right)}{(1 + 3C_m K_n) \left(1 + 2\frac{k_g}{k_s} + 2C_t K_n\right)} v \frac{\nabla T}{T}$$

where  $K_n$  is the Knudsen number, C and A are empirical constants,  $k_g$  is the gas conductivity,  $k_s$  is the aerosol conductivity and v is the kinematic viscosity. Since the near wall temperature gradient is typically not resolved (i.e. LES vs DNS), the temperature gradient is determined from the convective heat transfer:

$$\dot{q}^{\prime\prime} = k_g \nabla T = h(T_g - T_w)$$

$$\nabla T = \frac{h(T_g - T_w)}{k}$$

Turbulent deposition is a function of the dimensionless stopping distance,  $\tau^+$ , of the particle given by

$$\tau^+ = \frac{\rho_s {d_s}^2}{18\mu^2} \tau_w$$

Where  $\rho_s$  is the solid density,  $d_s$  is the mean diameter (definable by the user on &SPEC using the keyword MEAN\_DIAMETER.),  $\mu$  is the gas viscosity, and  $\tau_w$  is the wall shear stress obtained from the Werner-Wengle model. The deposition velocity is given by

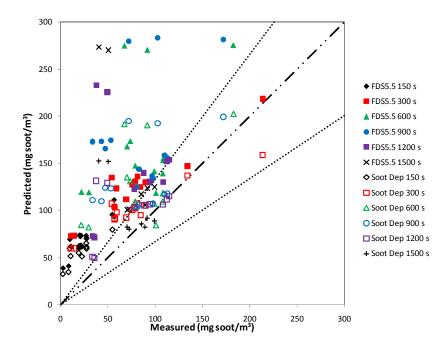
$$v_{turb \ dep} = v^+ u_{\tau}$$

where  $u_{\tau}$  is the friction velocity and  $v^+$  is the dimensionless deposition velocity given by:

$$v^{+} = \begin{cases} 0.086Sc^{-0.7} & \tau^{+} < 0.2\\ 0.00035 \ (\tau^{+})^{2} & 0.2 < \tau^{+} < 30\\ 0.17 & \tau^{+} > 30 \end{cases}$$

The regimes from top to bottom are diffusion regime, diffusion impaction regime, and inertiamoderated regime.

Adding this simple model reduced errors in predicting the soot obscuration in Benchmark Series 3 by 50 %. This can be seen in the figure below where solid symbols are without deposition and hollow symbols are with deposition.



#### 5.0 Minor Enhancements

#### 5.1 Droplet Evaporation

During the development of FDS v5 a series of verification cases were created for droplet evaporation. These cases revealed that there were errors in energy conservation associated with the droplet evaporation and that there were errors in the computed end state. Three contributing causes were identified: an incomplete accounting of the effect of evaporation on the divergence, inconsistencies between the liquid phase and gas phase enthalpies of the water, and overshoots in the evaporation that resulted in super-saturation.

Multi-Parameter Combustion Model for FDS

The FDS divergence equation is given below. Terms with 'b' subscripts represent divergence changes that result from bulk sources of mass (e.g. water vapor from evaporation). The first release of FDS v5 did not contain all of the terms related to bulk sources. This was a major contributor to the errors in the verification cases.

$$\nabla \cdot \mathbf{u} = \left( \frac{1}{\rho c_p T} - \frac{1}{\overline{p}_i} \right) \frac{D\overline{p}_i}{Dt} + \frac{1}{\rho} \left[ \dot{m}_b^{\prime\prime\prime} \frac{\overline{W}}{\overline{W}_b} + \overline{W} \sum_{\alpha} \frac{1}{W_{\alpha}} \left\{ \dot{m}_{\alpha}^{\prime\prime\prime} - \nabla \cdot \mathbf{J}_{\alpha} \right\} \right]$$

$$+ \frac{1}{\rho c_p T} \left[ -\sum_{\alpha} \Delta h_{\alpha}^0 \dot{m}_{\alpha}^{\prime\prime\prime} - \sum_{\alpha} h_{s,\alpha} \left( \dot{m}_{\alpha}^{\prime\prime\prime} - \nabla \cdot \mathbf{J}_{\alpha} \right) - \nabla \cdot \dot{\mathbf{q}}^{\prime\prime} - \dot{q}_b^{\prime\prime\prime} + \dot{m}_b^{\prime\prime\prime} \sum_{\alpha} Y_{b,\alpha} c_{p,\alpha} (T_b - T) + \frac{\dot{m}_b^{\prime\prime\prime}}{2} \left| \mathbf{u}_b - \mathbf{u} \right|^2 \right]$$

The divergence terms for bulk sources are:

$$\frac{1}{\rho}\dot{m}_b^{\prime\prime\prime}\frac{\overline{W}}{\overline{W}_b} + \frac{1}{\rho c_p T} \left( -\dot{q}^{\prime\prime\prime}{}_b + \dot{m}_b^{\prime\prime\prime} c_{p,b} (T_b - T) + \frac{\dot{m}_b^{\prime\prime\prime}}{2} |\boldsymbol{u}_b - \boldsymbol{u}|^2 \right)$$

From left to right these terms are divergence due to the change in average molecular weight, divergence due to convective and radiative heat transfer to the bulk mass, divergence related to the net gain or loss of enthalpy, and finally divergence related to the net gain or loss of kinetic energy of the bulk mass. A new divergence source term was created that included everything except for the kinetic energy term.

The third term in the bulk divergence is the change in enthalpy due to the addition of the bulk mass. In the case of water evaporation this enthalpy change is reflected as a heat of vaporization plus the enthalpy difference between the water vapor and the local gas. Previously FDS used thermophysical properties for the liquid water that were not consistent with the gas phase properties. That is summing the liquid enthalpy plus the heat of vaporization did not always equal the gas phase enthalpy at that temperature. This inconsistency resulted in errors in computing the third term. Corrections to the thermophysical properties eliminated this source of error. These changes are discussed in more detail in Section 5.3.

A final source of error came from the solution scheme for the droplet evaporation. Two ODEs representing the enthalpy and mass of the droplets are solved to obtain the evaporation rate. Using this evaporation rate the end of time step gas phase conditions (temperature, density, species, etc.) can be determined. Under conditions of rapid evaporation, using the ODE predicted evaporation over the entire time step could result in overshooting the mass of water vapor (i.e. based on the end of time step temperature the water vapor mass fraction could exceed 100 % relative humidity). Since FDS does not currently have a routine to condense vapor back into a liquid, this overshoot would remain in future time steps. A check was added to the droplet evaporation routine and if supersaturation occurs, the ODE is resolved using a smaller time step.

With these revisions errors of more than 10 % in the energy exchange between the liquid and the vapor were reduce to less than 1 %.

## 5.2 Enthalpy Diffusion

In the divergence equation above there is the term  $\nabla \cdot \dot{q}''$ . This term represents the divergence due to the transport of enthalpy via conduction, diffusion, and radiation. This term expands to:

$$\dot{q}^{\prime\prime} = -k\nabla T - \rho \sum_{\alpha} D_{\alpha} h_{\alpha} \nabla Y_{\alpha} + \dot{q}_{r}^{\prime\prime}$$

The middle term was not present in the original release of FDS v5. Omitting this term resulted in energy conservation errors that became more noticeable when improved thermophysical properties and improved species transport schemes were implemented. This term was added to FDS v5.

#### 5.3 Thermophysical Properties

The existing routines for computing enthalpy and specific heat of gas mixtures and liquids were changed to make use of data from the Joint-Army-Navy-Air Force (JANAF) Thermochemical tables where data was available. The JANAF tables provide a large database of compounds that can be added to FDS to support evolving user needs. Additionally, the JANAF tables contain properties of common liquids. The evaporation routines were modified to make calls to tabulated properties of the liquids. The liquid and gas phase tables were implemented so that zero enthalpy of a species was taken as the liquid enthalpy at the liquids freezing point. Published heats of vaporization were then used to set the 0 K enthalpy of the gas phase. These steps ensure consistence between the liquid and gas phases and avoid the errors in computing divergence that occurred prior to these changes

#### 5.4 Species Database

One of the goals in changes to species tracking was to support users interested in tracking toxicants. In applications such as rail car fires, plastics and foams used on the interior of rail cars can produce large quantities of irritant or toxic gases that could impact egress. Using these species on the &SMIX and &SPEC inputs requires the specification of molecular weights, viscosities, and specific heats. To reduce the burden on the user community, the 9 predefined species in FDS v4 was expanded to 36 species. Where it existed, both gas and liquid phase specific heat data was added to FDS along with molecular weights, the heat of vaporization (at the boiling point), boiling and freezing temperatures, and Lennard-Jones parameters for computing viscosity. The species are shown in the table below.

Species	Mol. Wgt.	Formula	σ	$\epsilon/k$	Liquid
	(g/mol)		(Å)	(K)	
ACETYLENE	26.037280	C <sub>2</sub> H <sub>2</sub>	4.033	231.8	
ACROLEIN	56.063260	C <sub>3</sub> H <sub>4</sub> O	4.549	576.7	Y
AIR	28.848523		3.711	78.6	Y
ARGON	39.948000	Ar	3.42	124.0	Y
BUTANE	58.122200	C4H10	4.687	531.4	Y
CARBON DIOXIDE	44.009500	CO <sub>2</sub>	3.941	195.2	
CARBON MONOXIDE	28.010100	CO	3.690	91.7	Y
ETHANE	30.069040	C <sub>2</sub> H <sub>6</sub>	4.443	215.7	Y
ETHANOL	46.068440	C <sub>2</sub> H <sub>5</sub> OH	4.530	362.6	Y
ETHYLENE	28.053160	C <sub>2</sub> H <sub>4</sub>	4.163	224.7	Y
FORMALDEHYDE	30.025980	CH <sub>2</sub> O	3.626	481.8	Y
HELIUM	4.002602	He	2.551	10.22	Y
HYDROGEN	2.015880	H <sub>2</sub>	2.827	59.7	Y
HYDROGEN BROMIDE	80.911940	HBr	3.353	449.0	Y
HYDROGEN CHLORIDE	36.460940	HCI	3.339	344.7	Y
HYDROGEN CYANIDE	27.025340	HCN	3.63	569.1	Y
HYDROGEN FLUORIDE	20.006343	HF	3.148	330.0	Y
ISOPROPANOL	60.095020	C <sub>3</sub> H <sub>7</sub> OH	4.549	576.7	Y
METHANE	16.042460	CH <sub>4</sub>	3.758	148.6	Y
METHANOL	32.041860	CH <sub>2</sub> OH	3.626	481.8	Y
N-DECANE	142.281680	C10H22	5.233	226.46	
N-HEP TANE	100.201940	C7H16	4.701	205.75	Y
N-HEXANE	86.175360	C <sub>6</sub> H <sub>12</sub>	5.949	399.3	Y
N-OCTANE	114.228520	C8H18	4.892	231.16	Y
NITRIC OXIDE	30.006100	NO	3.492	116.7	Y
NITROGEN	28.013400	N <sub>2</sub>	3.798	71.4	Y
NITROGEN DIOXIDE	46.05500	NO <sub>2</sub>	3.992	204.88	Y
NITROUS OXIDE	44.012800	N <sub>2</sub> O	3.828	232.4	Y
OXYGEN	31.998800	O <sub>2</sub>	3.467	106.7	Y
PROPANE	44.095620	C <sub>3</sub> H <sub>8</sub>	5.118	237.1	Y
PROPYLENE	42.079740	C <sub>3</sub> H <sub>6</sub>	4.678	298.9	Y
SOOT	12.010700	С	3.798	71.4	
SULFUR DIOXIDE	64.063800	SO <sub>2</sub>	4.112	335.4	Y
SULFUR HEXAFLUORIDE	146.055419	SF <sub>6</sub>	5.128	146.0	
TOLUENE	92.138420	C <sub>6</sub> H <sub>5</sub> CH <sub>3</sub>	5.698	480.0	Y
WATER VAPOR	18.015280	H <sub>2</sub> O	2.641	809.1	Y

#### Multi-Parameter Combustion Model for FDS

## 5.5 Input File Readability Improvements

From FDS v2 to the current alpha version of FDS v6, input processing has grown from 6,000 lines of code to over 15,000 lines of code. This growth has occurred from the addition of new features, the addition of new output quantities, and the expansion of built-in property data. With this expansion, being able to clearly interpret the input file was becoming more difficult. This increases the time to perform a QA check of an input file, increases the likelihood of user errors, and just generally adds to the difficulty of reading the input file.

One contributing factor was that inputs related to a specific phenomenon were split over multiple namelist groups. For example in FDS v5 the background gas species was defined on the &MISC line and all other gas species were defined on the &SPEC lines. Additionally there was a lack of consistency between how inputs were specified. For example mass fluxes of species on a &SURF line were identified solely by the order in which they were specified on the &SPEC lines (inputs that might not be visible on the screen while viewing the &SURF line). As a second example gases produced by solid phase reactions were identified using a different keyword and input format than gases produced by gas phase reactions. In moving towards FDS v6, a number of changes have been made to the FDS inputs to make them more consistent and to make the locations of inputs more logical.

## 5.5.1 Relocated Inputs

One set of readability improvements involved moving inputs to more appropriate namelist groups. The definition of the background species was removed from &MISC and instead the user now denotes a &SPEC or &SMIX as the BACKGROUND. The specification of liquid properties on &PART was moved to &SPEC to keep all species properties together. A number of other parameters on &MISC were moved to more directly related namelist groups (for example the flag RADIATION to turn on or off the radiation solver was moved to &RADI the input group for controlling the radiation solver).

## 5.5.2 Input Consistency

For many input groups in FDS v5, an input defined on another namelist was defined as NAMELIST\_ID. For example if a &DEVC was to be used to control a &VENT, the input DEVC\_ID was used. This clearly indicates what is being referred to on the inputs. Not all inputs were treated in this manner. For example if a user was specifying a MASS\_FRACTION boundary condition for a &SURF, the user merely listed the values for each species in the order they were defined on the &SPEC line. If a species was not being used, either a zero had to be specified or the array had to be explicitly defined with indices for each value. An input such as

&SURF ID='inlet', VEL=-1, MASS\_FRACTION=0.0,0.1,0.0,0.9/

is not easily understandable and in a long input file, especially if the &SPEC lines are not visible at the same time. Similarly when solid phase reactions were being used, a series of keywords were used to identify fuel, gas, or solid phase species being produced without a clear tie (in terms of a QA reviewer) to &SPEC or &MATL inputs. FDS inputs were modified to require the use of SPEC\_ID and MATL\_ID to denote inputs. Using this approach, only species actually being produced or removed by a namelist need to be specified (i.e. no zero values need to be given). This avoids errors that result by not properly ordering inputs to match the order of &SPEC lines and makes it clear without having to refer back to the &SPEC lines or &MATL lines what is being specified.

## 5.5.3 Defining Reactions

A number of input changes were made to the specification of reactions to improve the readability of the inputs and to allow for additional error checking by FDS.

For the typical FDS user, using the simple chemistry approach (e.g. inputs of C, H, O, N, CO\_YIELD, and SOOT\_YIELD), little has changed other than two input changes. The first is that the species OTHER is no longer available as part of the simple chemistry input. If a user wishes to track additional species, then those species will have to be defined explicitly. The second change is that users will have to specify a &REAC input and a FUEL for the reaction. There will no longer be the default mixing controlled reaction of propane combustion. Many users never defined an explicit &REAC input leading to simulations where the oxygen consumption and species production was not appropriate for the actual fuel being burned.

To enable FDS to guarantee both mass and element conservation in reactions, a periodic table was added to FDS. When specifying a &SPEC input or when defining the FUEL for use with simple chemistry, a user can now specify a FORMULA. FDS will parse the formula to determine the atom counts of the elements given in the FORMULA. Element names are case sensitive and follow the IUPAC nomenclature. Examples of FORMULAs are given below (both are heptane):

FORMULA='C7H16' FORMULA='CH3(CH2)5CH3'

Note that ()s can be used in the formulas. For pre-defined species, there is no need to specify the FORMULA.

Specifying a FORMULA allows FDS to compute the molecular weight of a species and to track the atom counts for each species.

In addition to the FORMULA keyword, the keyword EQUATION was also added to the &REAC input. This keyword provides an alternate and more easily read method of specifying the reaction stoichiometry. For example the following inputs would specify the same chemical reaction (appropriate &SPEC lines would be needed):

```
&REAC FUEL='PROPANE', SPEC_ID='PROPANE', 'OXYGEN', 'CARBON DIOXIDE', 'WATER VAPOR', NU = -1, -5, 3, 4, .../
```

&REAC FUEL='PROPANE', EQUATION='PROPANE+5\*OXYGEN=3\*CARBON DIOXIDE+4\*WATER VAPOR',.../

&REAC FUEL='PROPANE', EQUATION='C3H8+5\*O2=3\*CO2+4\*H2O', .../

## 5.6 New Output Quantities

The following new output quantities (and other &DEVC inputs) were added:

Quantity	Unit	Description
AIRCOIL HEAT EXCHANGE	kW	Heat exchange for an &HVAC AIRCOIL. Requires AIRCOIL_ID.
AVERAGE SPECIFIC HEAT	kJ/kg/K	$\bar{c}_p$
CONDUCTIVITY	W/m/K	k (gas phase)
DRY		Logical flag modifier for MASS FRACTION or
		VOLUME FRACTION. Removes WATER VAPOR
		prior to computing output.
DUCT VELOCITY	m/s	Flow velocity in a duct. Requires DUCT_ID.
DUCT TEMPERATURE	°C	Temperature of flow in a duct. Requires DUCT_ID.
DUCT MASS FLOW	kg/s	Total mass flow in a duct. Requires DUCT_ID.
DUCT VOLUME FLOW	$m^3/s$	Volumetric flow in a duct. Requires DUCT_ID.
DUCT MASS FRACTION		Mass fraction of a species in a duct. Requires
		DUCT_ID and SPEC_ID.
DUCT VOLUME FRACTION		Volume fraction of a species in a duct. Requires
		DUCT_ID and SPEC_ID.
DUCT DENSITY	kg/m <sup>3</sup>	Density of flow in a duct. Requires DUCT_ID.
ENTHALPY	kJ/m <sup>3</sup>	Н
FILTER LOADING	kg	Mass loading of a filter. Requires FILTER_ID
		and SPEC_ID.
FILTER LOSS		Flow loss through a filter. Requires FILTER_ID.
NODE DENSITY	kg/m <sup>3</sup>	Density of a duct node. Requires NODE_ID.
NODE MASS FRACTION		Mass fraction of a species in a duct node. Requires
		NODE_ID and SPEC_ID.
NODE PRESSURE	Pa	Pressure at a duct node. Requires NODE_ID.
NODE PRESSURE	Pa	Pressure difference between two duct nodes.
DIFFERENCE		Requires NODE_ID(2).
NODE TEMPERATURE	°C	Requires NODE_ID.
NODE VOLUME FRACTION		Volume fraction of a species in a duct node.
		Requires NODE_ID and SPEC_ID.
NORMAL VELOCITY	m/s	Normal velocity at a wall cell.
SOLID CONDUCTIVITY	W/m/k	k <sub>s</sub> Requires DEPTH.
SOLID SPECIFIC HEAT	kJ/kg/K	c <sub>p,s</sub> Requires DEPTH.
SMOOTHING_FACTOR		Performs an exponential smoothing on the output
		of a &DEVC. Smoothed <sub>n</sub> = $SF * Smoothed_{n-1} +$
		(1 - SF) * CurrentValue
SPECIFIC ENTHALPY	kJ/kg	h

## 5.7 &RAMP DEVC\_ID

A request from multiple users was to be able to control a ramp using a quantity other than time. The input keyword DEVC\_ID was added to &RAMP. When this keyword is specified, the ramp will be evaluated using the specified device rather than time. In this manner the flow through a vent could, for example, be made temperature dependent.

## 5.8 &SURF NET\_HEAT\_FLUX

FDS had inputs to allow the user to specify a convective heat flux and a radiative heat flux at a solid surface. These inputs were independent of one another. An additional key word, NET\_HEAT\_FLUX, was added to allow the user to specify a total heat flux that is a combination of convective and radiative. Additionally the ADIABATIC boundary condition was modified to be equivalent to NET\_HEAT\_FLUX=0. The net heat flux is obtained by iterating the equation:

$$\dot{q}^{\prime\prime} = h(T_g - T_w) + \dot{q}^{\prime\prime}_{rad,in} - \epsilon \sigma T_w^{4}$$

until a solution is obtained.

## 5.9 Temperature Dependent Species Properties

While there are many more predefined species in FDS v6, there are still a much larger number that are not predefined. Previous versions of FDS only allowed the user to specify a single value for the specific heat, conductivity, or viscosity of a species. The &SPEC inputs were expanded to allow the user to specify temperature dependent &RAMPs for these quantities.

## 6.0 User Support

User support was provided via the GoogleCode issue tracker and the GoogleGroups discussion forum. 296 issues were addressed during the three year grant period and 624 postings were made to the discussion forum. A summary is provided in Appendix C for the issue tracker and Appendix D for the discussion forum.

## **APPENDIX A: FDS Releases**

Below is a summary of the FDS releases for the 2008-2011 reporting period.

- Version 5.5.3 October 29, 2010: SVN Revision 7031 Version 5.5.2 – September 3, 2010: SVN Revision 6706 Version 5.5.1 – June 23, 2010: SVN Revision 6385 Version 5.5.0 – April 6, 2010: SVN Revision 6006 Version 5.4.3 – December 4, 2009: SVN Revision 5210 Version 5.4.2 – October 19, 2009: SVN Revision 4957 Version 5.4.1 - September 10, 2009: 4697 Version 5.4.0 – September 1, 2009: SVN Revision 4629 Version 5.3.1 – April 8, 2009: SVN Revision 3729 Version 5.3.0 – January 30, 2009: SVN Revision 3193 Version 5.2.5 – December 10, 2008: SVN Revision 2828 Version 5.2.4 – November 11, 2008: SVN Revision 2651 Version 5.2.3 – October 16, 2008: SVN Revision 2514
- Version 5.2.2 October 16, 2008: SVN Revision 2510
- Version 5.2.1 September 15, 2008: SVN Revision 2376

## **APPENDIX B: Source Code Commits to GoogleCode**

The table below contains the SVN log entries for the 435 code commits by the author during the 2008-2011 reporting period. Under SVN each commit is assigned its own version number. A single commit may contain multiple files.

SVN	User Reported Summary [sic]			
	FDS Source: Change DZ to DZZ for divergence term to avoid potential future conflict with			
8958	global DZ variable.			
8947	FDS Source: prevent infinite loop for zeroth order reactions			
8922	FDS Source: Fix RK2 ODE solver			
	FDS Source: Fix soot_deposition error when SIMPLE_CHEMISTRY is set and a background			
8920	SOOT value is set. Issue 1474			
8919	FDS Source: HIDE/SHOW SMV time incorrect when CTRL is being used.			
8896	Correct FORMULA for He			
	FDS Source: Fix bug in temp update in part.f90. Add dc_p/dt terms to temp updates in			
8880	hvac.f90.			
8879	FDS Documentation: Add new HVAC output QUANTITIES for filters and aircoils			
8878	FDS Source: Fix sign on FIXED_Q for AIRCOIL			
8877	FDS Documentation: Updates to User Guide HVAC discussion for filters and aircoils			
8875	FDS Source: Fixes to FILTER for HVAC. Addition of AIRCOIL to HVAC.			
8860	FDS Source: Add filtration to HVAC.			
8858	FDS Documentation: Update mass chapter from Y to Z			
	FDS Source: Improved thermophoretic and turbulent deposition. Additional inputs on SPEC			
8856	for aerosol.			
	FDS Source: Remove NEW_COMBUSTION and old routine. Re-enable SOOT_DEPOSITION			
8851	and being making deposition generic (allow			
	FDS Source, FDS Documentation: Cleanup RAMP DEVC example per Issue #1453. Add			
8842	SMOOTHING_FACTOR to DEVC for smoothing ou			
8786	FDS Documentation: Update to HVAC section.			
	FDS Source FDS Documentation: Update namelist tables in guide, fix alphabetization in			
8785				
	FDS Documentation: Minor edits to chapter 2 of the Tech Guide including changing Y to Z			
	where appropriate			
	FDS Documentation: Lumped species text at start of mass transport			
8774	FDS Documentation: Minor edits.			
	FDS Documentation: Minor edit to CMP to make version number description consistent with			
	remainder of CMP.			
8767	Fix deletion of second half of IF block for POROUS removal in check mass fraction			
8762	FDS Source: Add RAMP to DUCT for VOLUME_FLOW			
8747	FDS Documentation: Updates to HVAC writeup and fix ROTATION			
8745	FDS Documentation: Update User's Guide for deletion of POROUS			
	FDS Source FDS Verification: Remove POROUS and change jet_fan.fds to use HVAC			
8742	FDS Source FDS Verification: HVAC leakage fix. Update door_crack verification case			
	FDS Source Verification: Update leak_test cases and exact solution, tweak to fan curve			
8738	relaxation.			

SVN	User Reported Summary [sic]
8731	FDS Verification: Update plot bounds for fan test
	FDS Source, FDS Verification: HVAC fixes. Adjust FAN definitions to get good analytic solution
	FDS Source: HVAC leakage fix
	FDS Verification: Adjust verification cases for recent HVAC fixes
	FDS Source: Additional bug fixes to HVAC routines
	FDS Source: Fixes to HVAC routines
	FDS Source: Fixes to HVAC routines. Improve error messages for QUANTITY errors.
	FDS Documentation: Fix LEMTA figure callout in Heat_Flux_Chapter.tex
	FDS Source: Fix error in FUEL MW when user overrides C,H,N,O values for
8562	SIMPLE_CHEMISTRY
	FDS Source: Fix Issue #1431 not initializing ATOMS for SOOT species when user defined.
-	FDS Verification: Fan curve error
	FDS Source: Fix HVAC BC error for leakage flows
	FDS Source: Fix dimension error
	FDS Source: fixed variable dimension
	FDS Source, Documentation: Fix error in diagnostic for atom balance error, add REAC inputs
8531	CHECK_ATOM_BALANCE, REAC_MASS
-	FDS Source: Fix pointer error
-	FDS Source: Missed committing file with earlier commit on H_V fix
	FDS Source: Fix for H_V calc for user defined liquids
	FDS Source, FDS Verification: Minor tweaks to water evaporation exact solutions, fix PDPA
8302	devc in _3, get correct MW_RAT
-	FDS Verification: Remove duplicate leak_test_2 writeup.
	FDS Verification: Fix HVAC figure reference for ASHRAE #7
	FDS Verification: Re-add HVAC figure
	FDS Source: Fix formula error for Soot
	FDS Source: Fix error in setting MW when a FORMULA is given on SPEC
	FDS Source: Change SPECIFIC_ENTHALPY to REFERENCE_ENTHALPY and set the default to be
8187	SPECIFIC_HEAT * REFERENCE_TEMPERATU
-	FDS Documentation: Fix example for SMIX for AIR
	FDS Documentation: Updates to combustion writeup
	FDS Source, FDS Documentation: Remove unused variables from REACTION_TYPE. Improve
8171	commenting in fire.f90. U Guide upd
	FDS Source : Fix formulation of GET_AVERAGE_SPECIFIC_HEAT_DIFF
	FDS Source: Array bound error.
	FDS Source: Change ZZ to ZZP.
	FDS Source: Add back GET_AVERAGE_SPECIFIC_HEAT_DIFF for speedup in divg.f90
	Add comments to extinction routine
	Fix bug in extinction routine.
	FDS Documentation: Fix spelling error
	FDS Source: Issue #1386. Fix droplet properties when user specified
	FDS Source: declaration error
	FDS Source: Explicit Euler for multiple, simultaneous reactions. Add N_T to REAC
8156	(temperature exponent for rate)
2200	

SVN	User Reported Summary [sic]
8153	FDS Source: fix sign error in EXTINCTION routine
8152	FDS Source: Fix error in prior fix to HDIFF terms
	FDS Source: Re-add enthalpy difference to divg removed in SVN 7988
	FDS Source: Explicit Euler for Arrhenius reactions. Add reaction A,E to .out file. Fix
8145	SEARCH_INPUT_FILE so it it look
8142	FDS Source: missed file in prior commit
8141	FDS Source: Numerical precision for difference comparisons.
8139	FDS Source FDS Verification: Fix bug in ODE_EXACT, adjust NU's in methane_flame_primitive
8138	FDS Verification: Tweak to methane lumped case
8137	FDS Source: bypass atom balance for simple chemistry
8136	FDS Source: Adjust HRRPUA , MLRPUA to limit to one reaction
	FDS Source + FDS Verification: Adjust SMIX definition. Add atom counts for simple chemistry
8135	to species mixture array
8133	FDS Source: adjust SPECIES(SOOT_INDEX)%ATOMS for SOOT_H_FRACTION
	FDS Source+Documentation: Creation of generic combustion routine. Currently only does
8132	the exact solution using the prev
8102	FDS Source: Fix abbreviations for HCl and HBr.
	FDS Source: Split READ_HVAC into READ_HVAC and PROC_HVAC. Reorder processing in
	read.f90.
8077	FDS Source: Fix error for multiple PART classes with the same species
	FDS Source: Fix calling order in read.f90 due to adding of RAMPs for SPEC. Fix undefined var
	error in GET_QUANTITY
	FDS Source: Remove GAMMA from PART.
	FDS Documentation: Updates for moving liquid data from PART to SPEC
8058	FDS Verification: Remove DENSITY from PART inputs
	FDS Source: Add default liquid densities to predefined species. Remove default value for
	DENSITY and DENSITY_LIQUID. A
8051	FDS Source: Fix FORTRAN non-standard usage and line length
	FDS Source: Remove H2_YIELD from REAC, fix undefined in data.f90 and func.f90, move
8050	liquid properties from PART to SPEC
0045	FDS Source: Add RAMP_CP,RAMP_CP_L,RAMP_MU,RAMP_K,and RAMP_D to SPEC. Begin
	moving PART liquid data to SPEC (old PART lo
	FDS Documentation: User Guide update for FORMULA and IDEAL
	FDS Source: Remove unused variables, fix alignment error for FORMULA
	FDS Source: Add parsing of chemical formula for SPEC and REAC
8034	FDS Source: Clean up HOC calc for IDEAL
0022	FDS Source: Get IDEAL working, fix N2 calc for SPECIES_MIXTURE(2), add HYDROGEN to
	SPECIES_MIXTURE(2)
	FDS Source: Fix typo
	FDS Verification: Fix PDPA outputs and change XYZ to XB for VOLUME MEAN FDS Validation: Input changes for modified species
/942	FDS Source: Fix HUMIDITY setting of SS%YY0 FDS Source, FDS Verification: Fix to Z2CP, Z2CBPAR, calc of dump for k, slight tweak to
70/1	water_evaporation_1 exact soluti
/93/	FDS Source: fix usage of I_FUEL and I_WATER

SVN	User Reported Summary [sic]
	FDS Source, FDS Documentation: Updates to User's Guide. Make SPEC input variables
	consistent with Guide
7935	FDS Source: Fix bug in reading extra species when SIMPLE_CHEMISTRY is being used
	FDS Verification: correct WATER RADIATION LOSS to PARTICLE RADIATION LOSS
	FDS Source: Fixes to get FED_FIC working again.
	FDS Source FDS Verification: Fixes for verification suite errors.
	FDS Source: Fixes to verification case runtime errors
	FDS Source / FDS Verification: Change species framework to have SPECIES_MIXTURE be
	tracked species, add Y_INDEX (species
	FDS Source: Change N_GAS_SPECIES to N_TRACKED_SPECIES
	FDS Source: Add acrolein, NO. Alphabateize property case select blocks
	FDS Documentation: Update species table in User's Guide, add acrolein and NO and add
	chemical formula column
	FDS Source, FDS Documentation: Add CH2O, SO2, and N2O to database.
	FDS Documentation: Fix grammar and minor edits
	FDS Source, FDS Documentation: change LUMPED SPECIES ONLY to
	SMIX_COMPONENT_ONLY
	FDS Documentation: Updates to REAC, SPEC, and SMIX discussions
	FDS Source: Remove BACKGROUND_ONLY flag. BACKGROUND now has the meaning of
	BACKGROUND_ONLY.
	FDS Source: Minor tweaks to CO parameters in fire.f90 and use of actual diffusivity for
	simple chemistry with dns.
	FDS Source: GAS_PHASE_OUTPUT is indirectly RECURSIVE due to
	WAVELET_ERROR_MEASURE
	FDS Source: Fix supersaturation check in part.f90
	FDS Source: Issue 1333. Fix an inconsistency in computing the equilibrium water vapor in
	dump vs in part
	FDS Source: Issue #1333, fix error in getting gas mass fraction of evaporating species (wasn't
7711	accounting for species th
7685	FDS Source: Make units of INIT HRRPUV correct
7684	FDS Source: Missed committing two files for INIT HRRPUV
	FDS Source: Add HRRPUV to INIT. If set on any INIT no combustion is done, only the INIT
7683	value(s) are applied.
	FDS Source: Based on question in group, added quantities SOLID SPECIFIC HEAT and SOLID
7682	CONDUCTIVITY (both require DEPTH)
7647	FDS Documentation: Add NODE PRESSURE DIFFERENCE to U Guide
	FDS Source: Add QUANTITY NODE PRESSURE DIFFERENCE and modify ASHRAE 7 test cases to
7639	use new device
7587	FDS Source: Issue 1318 fix work array error in divg.f90
7586	FDS Source: Fix water vapor initial mass fraction error for simple chemistry with sprinklers.
	FDS Data_Processing: In Hamins_CH4_Average.f90, EOF is not a standard intrinsic function.
7577	Standard intrinsic function i
7564	FDS Source: Make HEAT FLOW consistent with KP calc in divg.f90
7557	FDS Source: Fix undefined variable error

SVN	User Reported Summary [sic]
7555	FDS Source: Fix typo
	FDS Source: Cleanup of CP routines. Add func for background only calcs. Replace H
7554	variables with CP in SPECIFIC_HEAT c
7553	FDS Source: Fix spelling error
	FDS Source: Fix fuel index in fire.f90 for SIMPLE_CHEMISTRY case when FUEL_INDEX is set in
7549	SPEC rather than REAC
	FDS Source: MASK added to to UVWMAX not a valid Fortran statement. Cannot use a logical
	value as a mask for a real numb
	FDS Source: Fix processing of HRRPUA when simple chemistry lumped species are redefined
	FDS Source: Fix error in SIMPLE_CHEMISTRY if lumped species components are redefined in
	LUMPED_ONLY mode
-	FDS Source: Fix inconsistent formulation for CPBAR in read.f90.
	FDS Verification: Fix error in helium2d.fds
	FDS Documentation: Update aspiration example case
	FDS Verification: Modify door_crack.fds to use HVAC FAN instead of SURF FAN.
	FDS Source: Fix error in DU%VEL(NEW) for a FAN with REVERSE=.TRUE.
7496	FDS Verification: Minor changes to inputs
7492	FDS Source: Upload new type.f90 with HOC_COMPLETE
	FDS Source+Verification: Add Y_CO2_INFTY and HUMIDITY to box_burn_away inputs. Fix
7488	error in Y_N2_INFTY calc for when HU
7487	FDS Verification: Fix error in aspiration input file
7486	FDS Verification: Fix error in Y_H2O column of water_evaporation.csv
7472	FDS Validation: Changes to FSE inputs to remove legacy outputs
7470	FDS Source: Remove code for legacy output names
7469	FDS Validation: Update output quantities and REAC line for Beyler_Hood cases
7468	FDS Source: Adjust fit to equilibrium vapor calc.
7467	FDS Documentation: Start adding new species and combustion material to Tech Guide
7465	FDS Documentation: User guide edits for new species routines
	FDS Source: Additional reorganization of read.f90 to read all species prior to reading
7455	reactions (eliminates second pass
7454	FDS Verification: Fixes to verification suite
7425	FDS Documentation: Begin of updates to User's Guide for new species
7421	FDS Source: fix bug in read.f90 when no H is defined for REAC.
7420	FDS Verification: tweaks to verification cases for new species routines
7419	FDS Source: Fix lower bound of PC% thermal properties
7418	FDS Verification: Add WATER VAPOR species to case
7412	FDS Source: Bug fixes for new species routines
7410	FDS Verification: Changes to particle drag
-	FDS Source: Bug fixes to new species routines
	FDS Verification: Fixes to errors in verification suite
	FDS Source: Source changes for read reorg.
	FDS Verification: changes to verification suite for reorg of read.f90 inputs.
	FDS Source: changes to input processing in READ. Removal of many MISC items to other
7398	inputs. Reorg to force SPEC and R
7388	FDS Source: Fixes to read processing and wall for new species

SVN	User Reported Summary [sic]
7387	FDS Verification: Changes to Verification cases for new species
7367	FDS Documentation: Begin adding SMIX and SPEC changes to User's Guide
7364	FDS Source: Fix TOLUENE formula error
	FDS Source: Issue 1292. Need to pass PSUM prior to first timestep when HVAC is being used
7363	with multiple meshes.
7358	FDS Source: Fix spelling error
7357	FDS Source: missing NO2 in GAS_PROPS
	FDS Source: Source cleanup. Begin removal of == and /= for REAL comparisons. Replace
7355	with ABS()<=ZERO_P and ABS()>=ZER
7353	FDS Verification: Updates to Verification Suite for new species inputs
7351	FDS Source: data.f90 line ending verify
7350	FDS Source: Add data.f90
	FDS Source: Addition of &SMIX keyword, creation of data.f90, overhaul of species tracking,
	cleanup of legacy IF (.EQ.,
7310	FDS Source: Additional fix to NET_HEAT_FLUX to avoid error when EMISSIVITY=0.
7309	FDS Source: Net heat flux error with no radiation
7301	FDS Source: fix bad merging of versions from previous update
	FDS Source: Changes to FHRR calc, janaf tables, computation of D_LAGRANGIAN, beginning
7300	of D_REACTION addition
	FDS Verification: Slight tweaks to isentropic test case. PART SURF was not adiabatic.
7282	Increased number of particles to
	FDS Source, FDS Documentation: Put AIT back in. Call AUTO_IGNITION_TEMPERATURE and
	document in User and Theory Manual.
	FDS Source: Fix undefined variable error in hvac.f90
	FDS Source: Undefined variable error EVAC_FDS6
	FDS Source: Fix recursive USE due to use of ANGLE_INCREMENT in func.f90
	FDS Source: Fix recursive USE due to use of angle_increment in func.f90
	FDS Verification: Moving ashrae7 to verification
-	FDS Validation: Move ashrae7 to verificaiton suite
	FDS Validation: Adding ASHRAE sample problem 7
	FDS Documentation: Updates to HVAC input definitions in User's Guide
	FDS Verification: HVAC Verification writeup and scripts
7171	FDS Verification: Add SVN number to inputs
	FDS Source: Fan TAU fix, additional verification documentation. Change chod_hrr.csv to Pa
	from atm.
	FDS Source: Fix to FDS6 BC for HVAC or leakage
	FDS Verification: Inputs, exact outputs, smokeview scripts fort HVAC test cases
	FDS Verification: Begin adding HVAC verification
	FDS Verification: HVAC Verification Inputs
	FDS Validation: ASHRAE Validation inputs
	FDS Documentation: Updates to HVAC writeup
	FDS Source: Additional fix for #1262.
7154	FDS Documentation: Issue #1221, clarify definition of columns in chid_hrr.csv file.
	FDS Source: Issue 1262 - Add calc for QRADIN and QRADOUT for OPEN_BOUNDARY. Fix
/153	undefined variable in turb.f90

SVN	User Reported Summary [sic]
7152	FDS Source: Remove TAU_CHEM from local list as it is a global in cons.f90.
7150	FDS Source: Undefined variable. Keyword substitution fix.
7149	FDS Source: Uninitialized variable error in hvac.f90
	FDS Source: HVAC changes: various bug fixes, multiple mesh support, leakage now in HVAC
7146	solver, and MPI calls added (not
7143	FDS Source: Undefined variables fixes
	FDS Source: Undefined variable error. BLOW/SUCK check for material reactions. Change
7142	READ_ZONE location to before HVAC
7131	FDS Source: Remove COMBUSTION2 flag
7107	FDS Source: Make VEL_CHAR for DT independent of meshing
7060	FDS Source: typo fix
7059	FDS Source: Issue #1247. Minor typo in read.f90 reported by romboudvdw
7031	FDS Source: Make FHRR in UPDATE_HRR consistent with U Guide
7012	FDs Verification: Issue 1236. Fix "ideal" file.
	FDS Verification: Issue #1236. Modify aspiration case. Previously specified inlet and outlet
	condition in error.
	FDS Source: Set SPECIES_BC_INDEX to SPECIFIED_MASS_FRACTION when
	MASS_FLUX_TOTAL < 0.
	FDS Source: Fix MASSFLUX sum to include background flow.
	FDS Documentation: Adding HVAC to User's Guide
	FDS Documentation: Adding HVAC to User Manual
	FDS Documentation: Begin adding HVAC description to User and Theory Manual
	FDS Source: Add HVAC_BOUNDARY to mass.f90 wall routines
	FDS Source: Add ghost cell setting to HVAC_BC
	FDS Source: minor changes to hvac_bc for flux_limiter /= -1
	FDS Source: Fix array bounds error. Set RHOP to WORK8 rather than C_DYNSMAG
	FDS Source: Array bounds error fix in call to TEST_FILTER for RHOPHAT
	FDS Source: Issue #1198. Fix index for fuel mass fraction in old evap routine
	FDS Source: Shape conformance errors in turb. RHO is now -1: IBP1+1 which differs from
	most other global arrays from 0:
6781	FDS Source: Fix error in NU(O2_INDEX) when accounting for CO in two parameter.
<i>cc</i> 77	FDS Documentation: Issue # 1059. Updated guide for OVERWRITE and
	CHID='%INPUTFILENAME%'
	FDS Source: Issue #1059 by grgrgrknght. Added the logic for CHID='%INPUTFILENAME%' and added the keyword OVERWRITE to M
0074	FDS Source: Issue #1153. Extend thermophysical arrays to 0 K. Partial fix of the issue. Also
6672	fixed a couple of undefie
	FDS Source: Issue 1188 by mcgratta. unit label errors in JANAF functions
	FDS Source: Issue 1190 by crogsch. undefined variable error in divg.f90
	FDS Source: speed up following changes from timing test
	FDS Source: speed up following changes from timing test
	FDS Verification: Uncommit output files
	FDS Source: fix typo
	FDS Source: Issue #1154. Infinite loop in droplet routine. A mix of not doing linear interp on
	the enthalpy and havin
0575	

SVN	User Reported Summary [sic]
6554	FDS Source: Add GET_REV to scrc.f90
6517	FDS Verification: Force gamma to 1.4 for all temperatures for isentropic test cases
	FDS Source: background thermodata units adjusted twice in /misc/ and in /spec/; removed
6516	adjustment from /misc/
6344	FDS Source: Issue 1120, fix unit variables in particle_class_type.
6343	FDS Verification: N_REACTIONS was a real number.
	FDS Source: Issue 1120 - add error trapping for PART to make sure all properties are set if
6342	JANAF lookup is not being do
6226	FDS Source: tuning of new evap. Make use of mixture fraction D for DNS.
6224	FDS Source: Fix bad commit
6223	FDS Source: Issue 1094, new evap routine. enbaled with NEW_EVAP on MISC.
6204	FDS Source: Add RN%AIT to COMBUSTION_MF
	FDS Source: Issue 1076, fix output of MASSFLUX(IW,:) when desired species is part of a
6192	lumped species (e.g. Z1, Z2)
6112	FDS Source: Correct KP calc for LES
6111	FDS Source: Remove a debug printout
	FDS Source: change kp in divg for LES + add new extinction to combustion_mf (both linked to
6110	FDS6), tweaks to HVAC
6076	FDS Source: Issue 1063. Add call to CHECK_XB in READ_DEVC
	FDS Source: Edits to HVAC model. Add relaxation for fan pressure solution and velocity
6075	guess used in loss calc
	FDS Source: Add flags for THERMOPHORETIC_DEPOSITION and TURBULENT_DEPOSITION to
	&MISC
5988	FDS Source: Fix single species AVERAGE SPECIFIC HEAT output.
5957	FDS Source: Fix EQ vs EQV error in hvac.f90. Tuning change to wall.f90
	FDS Source: more HVAC updates. Add H_CHILTON_COLBURN for heat + mass transfer
5901	analogy. Modify thermophoretic soot depo
	FDS Documentation: Issue 1016, add to REAC input description that ETHYLENE is the default
5775	used for thermophysical proper
	FDS Source: Issue 1031, add RAMP_PART and TAU_PART to &SURF to control
	PARTICLE_MASS_FLUX
	FDS Source: Issue 1028. Change Y_O2_INFTY to be consistent with Standard Atmosphere.
	FDS Source: Issue #1022. Roll back prior fix and move correction to CONV_HRR calc.
	FDS Source: Issue #1022, adjust storage of enthalpy for vapors from liquid
	FDS Source: Reset point in EVALUATE_CONTROL after recursion call. Issue #1003
	FDS Source: Begin resolving Issue #1003
	FDS Source: Issue #1001. Begin process of nullifying pointers during initialization.
	FDS Source: Remove unused variables in hvac.f90
	FDS Source: Fix undefined error in dump.f90. Issue #999
5509	FDS Source: Issue #999. Undefined variable error in read.f90. Line length > 132 in main.f90
	FDS Source: Issue #999. Fix array out of bounds error and array mismatch error in
	PROC_SPEC
5504	FDS Source: Issue #999. Modify use of SOOT_INDEX in evac.f90
	FDS Source: Issue #999 Modify initialization of RCON_MF and the _INDEX variables for
5503	species to allow FED to work when

SVN	User Reported Summary [sic]		
	FDS Source: Issue#999 wasn't converting lower case MF species to upper case when		
	SPEC_ID was used previously was only c		
5456	FDS Source: Add GROUND_LEVEL to TMP_0		
	FDS Source: GROUND_LEVEL did not affect the pressure stratification. Modified so that i		
	ground level is not zero, that		
	FDS Source: comment out unused externals in mpis.f90. Fix some undefined variables.		
5442	FDS Source: NU(OTHER) error in read.f90		
5441	FDS Source: RN(1)%NU was not allocated the same as RN(>1)%NU for mixture fraction.		
	FDS Source: Fix NU_H2O error when no H is given on REAC		
	FDS Source: Issue 979. Prior commit was incorrect version of read.f90		
	FDS Source: Fix typo - 0 (number) rather than O (letter) - in read.f90. Reported by jukka in		
	Issue 979		
5421	FDS Source: Fix line length in type.f90		
	FDS Source: fix undefined variable error		
	FDS Source: Begin changes for Issue 972. Change Z species from fixed to allocated array.		
	FDS Source: Modify ITMP in part.f90 to prevent ITMP=0. Issue #910		
	FDS Source: Move H_EDDY into DNS if block so we don't use H_EDDY if DNS. Also add		
	complete calc for Cp so it is correc		
	FDS Source: Add error trapping for VOLUME FRACTION with MIXTURE FRACTION. Issue #963		
	FDS Documentation: Note not to use VOLUME FRACTION output for MIXTURE FRACTION,		
	Issue #963. Correct k/e in Lennard-Jone		
	FDS Source: Partially functional HVAC. Can couple multiple pressure zones using ducts with		
	loss / wall friction with no		
	FDS Documentation: Issue #962. Limit discussion of Z_f surface to FDS versions 2 - 4.		
	FDS Source: hvac network model. Currently only working in serial mode. Model is enabled		
	only if an &HVAC keyword is fo		
	FDS Source: add INTENT and units to JANAF functions		
5147	FDS Source: Verification case for unit changes Issue #919		
	FDS Source: Add logic to change DEVC%UNITS when a STATISTICS is used. Will stop		
5143	execution if an inappropriate STATISIST		
5142	FDS Source: removed a debug write		
5137	FDS Documentation: Add DEVC_ID to RAMP		
	FDS Source: Enable use of DEVC_ID for a RAMP. Replaces normal independent variable for		
5136	the RAMP with the output of the		
	FDS Source: Issue #940. Change fixed H_V in the HUMIDTY calc to use the JANAF		
	temperature dependent H_V. Apply to both		
	FDS Source: Issue #945 Fix file header for the mass file when an extra species is also in the		
5126	mixture fraction.		
	FDS Source: Add PDPA_NORMALIZE to &PROP to do a pure volume integration and not		
	weight by PDPA sensor volume. Modify wa		
	FDS Documentation: Update user's guide for changes to REAC and PART for evaporation		
	changes in 5056		
	FDS Source: fix uninitialized strings in read_prop. fix non-standard IF in turb.f90		
	FDS Souce: Fix unit variable error in read_reac in read.f90		
	FDS Source: Changes to data tables for liquid and gas properties. Changes to initialization o		

SVN	User Reported Summary [sic]			
	liquid properties. Allo			
4974	FDS Documentation: Add text on computing cp and h to tech guide and JANAF ref to bib			
	FDS Source: uninitialized variables in read.f90			
	FDS Source: Add check for unphysical gas temperature changes in the evaporation routines.			
4944	Force a subtime step when H_N			
	FDS Source: Change PC%DRAG_LAW to integer to conform to coding standard.			
	FDS Source: Fix typo in read and remove dead code in part			
	FDS Source: undefined variable and array alignment errors			
	FDS Documentation: Modify writeup of water_evaporation to allow for automatic updates.			
	FDS Source: Big fixes to water evaporation and addition of 1/GAMMA to D_VAP term.			
4873	Removal of fixed CP_H2O_LIQUID in fun			
4832	FDS Source: Fix line lengths for divg.f90. Possible source of Issue#880.			
	FDS Source: Fix enthalpy calc bug in combustion_mf2 found by Jukka V. and add AIT for			
4802	reaction.			
	FDS Source: updates to combustion2, use of analytic solution for single step and changes to			
4792	enthalpy calc for suppressio			
	FDS Verification: modified windows script. Run from verification directory as			
	run_verification %1 where %1 is the relat			
4636	FDS Verification: Windows bat file to run verification cases on a single processor.			
	FDS Source: Add back in breakup and wall particle temperature lines removed by error in			
4590	4136.			
	FDS Source: Add diffusive component to FHRR for VENTs that are OPEN or have a specified			
	velocity/flux. Issue #835			
	FDS Documentation: Bio updates			
	FDS Source: bug fix in tuning			
4535	FDS Source: tuning of velocity_bc, Issue #834			
	FDS Documentation: Add note on how to sum up multiple beam detector DEVC to get one			
4477	effective DEVC that spans multiple m			
	FDS Source: Change to specified mass fraction to ensure specified species are inserted when			
4424	they are equal to the ambien			
1201	FDS Source: Start of new routines for combustion. Not yet fully functional, hidden behind			
	COMBUSTION2 flag on MISC. 5t			
	FDs Validation: Fix case for Beyler in devc name			
	FDS Validation: Beyler hood cases FDS Validation: Beyler hood cases. FDS inputs, outputs, experimental, and post-process .f90			
	FDS Validation: Beyler hood cases. FDS inputs, outputs, experimental, and post-process .i90 FDS Source: Simplify PWT calc for spray distribution table.			
	FDS Source: Better approach for STRATUM using RN			
4293	FDS Source: With STRATUM based on NLP depending on number of drops being inserted,			
4292	closeness to NLPMAX, and number of pa			
	FDS Source: Added logic to set ACCUMULATE_WATER for a DEVC of AMPUA.			
	FDS Source: Fix ()'s in evac.f90 if statements. Fix bug from prior fix for Issue 91.			
7202	FDS Source: Missed fixing an enthalpy function in divg.f plus error in CBPAR calc for non-			
4176	mixture fraction. Addition of			
	FDS Source: Add USE SOOT			
	FDS Source: roll soot routines into wall.f90			
. 10 1				

SVN	User Reported Summary [sic]	
	FDS Source: Add WALLBC fix from Issue 469 to main_mpi. Add soot.f90 and COMBUSTION2	
4152	flag for combustion test routine	
	FDS Source: Issue #469. WALL_BC was being called before COMBUSTION (which changes the	
4145	YY array used by WALL_BC). Switc	
	FDS Documentation: Issue #606. Added note on usage of PERMIT_HOLE when a FALSE and	
4138	TRUE OBST overlap.	
	FDS Documentation: Add AVERAGE SPECIFIC HEAT for DEVC table, RECOUNT DRIP for	
4137	BNDF, and H_V_REFERENCE_TEMPERATURE for PA	
	FDS Source: JANAF Tables for cp + h, temp dependent h_v in part (and dump), new output	
4136	AVERAGE_SPECIFIC_HEAT, fix DRY lo	
	FDS Source: Cannot define a pointer to NULL in a variable declaration when used as	
3846	arguement in the subroutine call.	
	FDS Validation: Add O2 data from experiment. Simplify DEVC list for fds inputs	
	FDS Source: Issue 709, changes in read to allow user to specify a specific heat wound up with	
3814	a bad specific heat when n	
	FDS Documentation: Issue #705. Added note that not all text file formats are supported for	
3793	all OS+compilers.	
	FDS Source: Initialize M%KAPPA to KAPPA0 rather than 0EB (default for KAPPA0 is 0EB)	
07.12	FDS Documentation: Add SPECIFIC_HEAT and SPECIFIC_ENTHALPY to SPEC discussion and	
3617	inputs table	
	FDS Documentation: Fix spelling error SPECIFIC ENTHALPY	
	FDS Source: Change units of REFERENCE_TEMPERATURE on SPEC	
5010	FDS Source: Add SPECIFIC_HEAT, SPECIFIC_ENTHALPY, and REFERENCE_TEMPERATURE to	
3609		
	Data: Flip axes for FSE 2008 temperature plots	
	Data: Addition of NIST FSE 2008 to new validation file	
	Data: NIST RSE 1994 Tests, CO+ CO2 vs. HRR	
5541	FDS Source: Fix comment label for SOOT SURFACE DENSITY and speedup of PATH	
3534	OBSCURATION	
3334	FDS Documentation: Add SPECIFIC ENTHALPY and modify ENTHALPY to output QUANTITY	
3577	table (part of Issue #682)	
5522	FDS Documentation: Add SPECIFIC ENTHALPY and modify ENTHALPY to output QUANTITY	
3521	table (part of Issue #682)	
	fix legend for temperature	
	further fixes to FSE plots	
	partial fix to FSE plots	
	Attempt to add FSE to file	
	•	
	FDS Source: Corrections to GET_ routines for new array size, Issue 664	
3481	FDS Source: Fix for MW calc for Issue 664.	
2453	FDS Source: Make ALPHA in WALL_MODEL a non-parameter. Exponential causing compiler	
3457	difficulties. Fixed line length in v	
2455	FDS Source: Partial fix for Issue 664 reported by jukka. Also removed intent in for pointer in	
3455	evac.	
2445	FDS Source: Partial fix for Issue #672. If a HOLE used a different type of controller than	
	orginal OBST, the original i	
3441	FDS Documentation: Add more detail to the DEADBAND CTRL function description based on	

SVN	User Reported Summary [sic]			
	commments by jtrelles in Issue #6			
	FDS Source: Adjust loop cycle if statement for CP generation with mixture fraction and extra			
3393	3 species			
3392	FDS Source: Fix for Issue 657 reported by PLDHuynh. Error in N_SPEC_EXTRA counter.			
3386	FDS Documentation: extend T_END for water_evaporation.fds case			
3385	FDS Source: Additional changes to D_VAP calc.			
	FDS Source: New D_VAP term in part.f90. Correction to liquid enthalpy calc in dump.			
3335	Modified water_vaporation.fds test			
	FDS Documentation: Modification of water_evaporation to inlcude new PDPA and ENTHALPY			
3289	QUANTITIES			
	FDS Source: Changes to CP_BAR and ENTHALPY functions, and changes to droplet energy			
	balance for determining gas temperat			
	FDS Documentation: Correct water_evaporation test case and User's Guide writeup.			
	FDS Source: Fix Soot MW when doing finite rate.			
	FDS Source: Fix handling of SOOT in radi.f90 for a finite rate calc.			
	FDS Source: Fix error in not computing RHO_D for AEROSOL			
3010	FDS Documentation: This file was removed from revision control by mistake			
	FDS Documentation: Removing files from control that don't need to be in control (generated			
	by Tex)			
2992	FDS Documentation: Accidentally added some files to repository			
	FDS Source: Fix to GET_KAPPA (soot wasn't being handled correctly). Fix to background			
2991	species MU and K lookups.			
	FDS Source: Extend Z definitions to allow for SOOT_DEPOSITION (currently only if			
	CO_PRODUCTION=.FALSE.). Z_1 = fuel, Z_2			
	FDS Source: Fix output of thermophysical properties to CHID.out for extra species.			
2962	FDS Source: Add SPEC_ID capability to MASS FLOW			
2045	FDS Source: Add warning to read.f90 that units are kJ/kg/K iif a large (>10) specific heat is			
	entered for a material.			
	FDS Source: Init KP in divg.f90 to Y2K_C(ITMPA) to prevent div by zero in wall.f90.			
	FDS Source: Add revision variables to turb.f90			
	FDS Source: Fixed bug in creating Y2KAPPA for finite rate calcs.			
2900	FDS Source: Used MAX rather than MIN for ITMP limit.			
2007	FDS Source: Issue #590 reported by gforney. Fix loop check in read.f90 for gas props. Also			
	fix array temporary warning			
	FDS Source: Issue #589. Adjust parsing of SPEC_ID and QUANTITY in GET_QUANTITY_INDEX			
2803	FDS Source: Remove YY_SUM from main.mpi			
2061	FDS Source: Change how mass fractions, molecular weight, cp, etc are computed. Now no difference in mixture fraction vs			
	FDS Source: Add DEVC QUANTITY CONDUCTIVITY and add to table in U Guide			
2040	FDS Documentation: Issue #553. Add a caution to Section 8.4 about applying multiple layer			
2700	materials to an OBST.			
2759	FDS Source: Error in creation of _devc.csv file name when COLUMN_DUMP_LIMIT is .FALSE.			
2750	and N_DEVC=1. Issue#558 by user			
2759	FDS Source: Discovered bug in logic of TWO_BYTE_REAL routine. Wasn't creating integer per			
2726	the documented description			
2750				

SVN	User Reported Summary [sic]	
	FDS Documentation: Add an explanation of how RAMP_T is used to determine T_W to 8.5.2	
2699	of the User's Guide. Issue#541 re	
	FDS Documentation: Add that one may use XB with a DEVC that has STATISTICS. Issue#530	
2667	reported by grgrgrknght	
2661	FDS Documentation: Fix typo reported in Issue#505	
	FDS Source: Add NET_HEAT_FLUX to SURF. Issue #528. Computes wall temperature to	
2657	obtain specified NET_HEAT_FLUX using bo	
2643	FDS Source: Use cpbar in part.f90	
2628	FDS Source: Issue #519 fix. Removal of CP_GAMMA.	
	FDS Source: Add CP calc to UPDATE_HRR in dump.f90 rather than using CP_GAMMA. Solves	
2624	much of the error reported in Issu	
2622	FDS Source: Used YY rather than YYP in CP_MF in divg.f90.	
	FDS Source: Fix to Issue #520. Improperly defined Z_VECTOR for doing _state.csv file.	
	Reported by nishiki.	
	FDS Source: Change in device type for DRY	
2595	FDS Source: Fix undefined var error with DRY and SLCF/PL3D	
	FDS Source: Add keyword DRY to DEVC to do dry mass and volume fraction for mixture	
	fraction DEVC.	
	FDS Documentation: Additions to CM Plan	
	FDS Documentation: Further additions to CM Plan	
	FDS Source: Fix division by zero in CHECK_DENSITY and CHECK_MASS_FRACTION	
	FDS Documentation: Additions to CM Plan	
	FDS Documentation: Add skeleton of CM Plan	
2560	FDS Source: Fix some undefined variables in read.f90	
	FDS Source: CHECK_MASS_FRACTION didn't account for porous boundaries. Reported by	
2558	putouthefirenow in the discussion gro	
	FDS Documentation: Issue #508. Add a caution about using a Smokeview keyword as an ID	
2557	for a SURF.	
	FDS Documentation: Add a warning to the User's guide to not include the mesh boundaries	
	on &TRN? inputs. Reported by ct	
	FDS Source: Fixes error in second cp loop, Issue #501 by jukka.vaari.	
2482	FDS Source: Add WARNING when DEVC not in bounds of any mesh.	
2404	FDS Source: Add error trapping for using a CTRL as input to a CUSTOM CTRL. Issue #486 by	
2481	dntra2.	
2475	FDS Source: Add Argon CP to CP calc in read.f90 per request of Jukka Vaari	
2442	FDS Source: in read.f90 a DEVC with XB had IOR forced to 1,2,or 3. User couldn't set	
	negative IOR. Bug found by jouton	
	FDS Documentation: Added NORMAL VELOCITY to output quantity table.	
2431	FDS Documentation: Fix dy to "script d" y in Eq. 6.7. Reported by J. Trelles.	
2240	FDS Documentation: Change aspiration test case to greatly reduce dependence on flow	
2340	solver or combustion model.	
7011	FDS Source: Modify reaction type definition and the get_xxx mixture fraction functions in	
2311	prep for generalizing mixture	

## **APPENDIX C: Issues Addressed**

The table below is a listing of the 291 issues in the online issue tracker that the author participated in the resolution of during the 2008-2011 reporting period. Each issue is assigned a unique ID number for tracking purposes.

ID	Туре	Status	User Reported Summary [sic]
1479	Defect	Verified	Radiation and Energy Balance
1474	Defect	Verified	simple vs non-simple chemistry for soot with no flow at all
1471	Defect	Verified	edit colorbar dialog crashes smokeview
1467	Defect	Invalid	Spurious generation of He
1459	Defect	Verified	smoke3d seems too thick
1454	Defect	Accepted	Particles move up when they should not
1453	Enhancement	Fixed	Enhancement request - variable speed fan
1449	Defect	Verified	Latest smv build displays no SLCF data
1445	Defect	Verified	multi-slice when planes differ slightly
1444	Defect	Accepted	part.f90 BLOCK_VOLUME doesn't accout for OBST
1437	Defect	Accepted	Stack Effect example in User's Guide different from actual case
1433	Defect	Closed	TMP_EXTERIOR for open vents creating forced velocity
1431	Defect	Fixed	SMIX and Soot
1420	Defect	Verified	HRR and sprinkler
1419	Defect	WontFix	Issue with pressure
1402	Defect	Verified	HRR: RAMP function and different grid size
1400	Defect	Verified	CONV_LOSS and HRR: Water Mist case
1395	Defect	Fixed	Cup_Burner processing script not working
1393	Defect	MoreInfo	HVAC not working in Linux version
1391	Defect	Duplicate	fds dies with pointer fault.
1390	Defect	Closed	problems with evacuation cases
1386	Defect	Started	Radiation absorption verification case not working
1383	Defect	Verified	AVG_DROP_TMP becomes very large in part.f90
1378	Defect	Verified	create_remove.fds and smv SVN-7457
1375	Defect	Verified	conformance error in SPRAY_ANGLE_DISTRIBUTION
1373	Defect	Duplicate	Differences between DEVCs for burning rate
1371	Defect	Verified	the jet fire plume not in the right direction, it deflected quickly
1370	Defect	AltInputs	Problem with opening of a window
			Difference between burning rates in CHID_hrr.csv vs.
1369	Defect	AltInputs	CHID_devc.csv
1356	Defect	Started	scrc.f90 does not compile
1347	Defect	New	Creation of mass
1340	Defect	WontFix	Picture filename - Smokeview
1333	Defect	Started	Water droplets evaporation
1327	Defect	Started	DNS combustion does not burn
1322	Defect	WontFix	FDS 5.5.3: problem with "pressure zones" test
			Sidewall sprinklers boost heat flux on wall, but cools off
1318	Defect	Verified	temperature
1312	Defect	WontFix	helium_2d case does not run with SPEC_ID parameter

ID	Туре	Status	User Reported Summary [sic]
1306	Defect	Fixed	water_evaporation verification case
1305	Defect	Verified	aspiration_detector verification case not working
1304	Defect	AltInputs	box_burn_away verification cases
1302	Defect	Verified	HVAC cases need to be checked
1301	Defect	Verified	fan_test and door_crack verification cases not working
1300	Defect	Started	energy budget verification cases are not working
1299	Defect	Verified	ice_water_ice verification case/script does not run
1298	Defect	Verified	pcm_slab verification case/script is not working
1292	Defect	Fixed	fan_test verification test broken
1289	Defect	Fixed	Try to model a stratified enviroment in the space
1276	Defect	WontFix	FDS5 don't run
1266	Defect	WontFix	Temperatures well above the adiabatic temperature
1262	Defect	Fixed	HRR: Incorrect calculation
1253	Defect	AltInputs	Ramp_Q problem
1247	Defect	Verified	possible typo
1246	Defect	WontFix	constant diffusivity coefficient
1245	Defect	WontFix	Two- and Four-way coupled
1244	Other	Fixed	Check write-up of HVAC in FDS Technical Reference Guide
1239	Enhancement	Verified	Remove WATER and FUEL logical parameters on PART line
1236	Defect	Verified	aspiration_detector verification test case not working properly
1232	Defect	Fixed	no pyrolysis if I add sprinkler
1225	Defect	AltInputs	problem with exhaust vent
1223	Enhancement	Closed	Access error issues
1221	Defect	Fixed	Conflicting Manual Text
1219	Defect	WontFix	HRR values if T_BEGIN is not "0"
1215	Defect	WontFix	Different HRR's
1212	Defect	AltInputs	FDS not recognized
1211	Defect	OnHold	Evaporation & Droplet temperature read-out difficulties
			Fire suppression - combination of ethanol_pan and flow_rate
1210	Defect	OnHold	doesn't work / delivers strange results
1199	Defect	WontFix	2D and 3D models comparison
1198	Defect	Fixed	Liquid evaporation model
1190	Defect	Fixed	Undefined TMP_G in divg.f90
1188	Defect	Fixed	JANAF_TABLE_LIQUID units
1183	Defect	UnVerified	Burn Away option
1182	Defect	UnVerified	No error message but calculation don't start
1181	Defect	Duplicate	Surface temperature of burning vents
1175	Defect	WontFix	Wall temperature of burning vents
1173	Defect	AltInputs	Stop after the second time step
1160	Enhancement	WontFix	Soot visibility colorbar should be flipped by default
1158	Defect	Verified	scrc.f90 not standard compliant
1154	Defect	Fixed	STOP STOP problem
1153	Defect	Closed	MELTING_TEMPERATURE not set
1149	Other	Invalid	Pool fire simulation
1143	Enhancement	WontFix	Improved Leak Area Compressible Flow Equation w/ F90 Code

ID	Туре	Status	User Reported Summary [sic]
1139	Defect	Closed	Numerical instability problem
1138	Enhancement	Accepted	Feature Request for Kill Function
1137	Defect	WontFix	Unexpected temperature decrease
1136	Defect	Verified	Initial Conditions: initial temperature < 0 °C failed
			Deviations in HRR between FDS simulated results and experiment
1126	Defect	WontFix	data
1124	Defect	MoreInfo	Effect of humidity
1120	Defect	Fixed	heptane fire with sprinkler (only prop_id and part_id) HRR to low
1117	Defect	AltInputs	Recording temperature at a solid surface
1115	Defect	AltInputs	Fan can't puch Air outside the tunnel.
1110	Enhancement	Invalid	Efficiency loss of fans
1104	Defect	MoreInfo	Water Fuel Sprays - Program Exception - access violation
1100	Defect	Invalid	output of volume flow rate at louvered vent
1097	Defect	WontFix	burning cube not heating on the side faces
1095	Defect	Verified	Autoignition temperature
1094	Enhancement	Closed	Verification case: ethanol evaporation in a Stefan tube
1092	Enhancement	Verified	Enhancement: Transient Thermocouple Model
			Different plume temperatures with EXTINCTION2 and 32 vs. 64
1090	Defect	Closed	bit mpi runs
1086	Enhancement	Closed	goto Time option
1082	Defect	WontFix	Ignore FDS comments
1081	Defect	AltInputs	Butane dispersion
1080	Defect	WontFix	Beginner in FDS
1077	Defect	WontFix	Similar files different solutions FDS5.5.3
1076	Defect	Verified	Water evaporation
1071	Defect	Duplicate	SMOKEVIEW - Nozzles are displayed in wrong direction
1070	Defect	Verified	SMOKEVIEW - Nozzles are displayed in wrong direction
1065	Defect	Invalid	loss of detectors
1063	Defect	Fixed	Negative obscuration from beams
			Feature request - Allow CHID to use a keyword indicating
1059	Enhancement	Fixed	filename should be CHID
1050	Defect	Verified	Water vapor from fuel inflow vent
			Final energy in closed adiabatic box not same for N2 injection
	Defect	Verified	mass which varies by rate only
	Defect	Verified	T_PARTICLE in .ini
1038	Defect	Verified	Numerical Instability with FDS 5.5.0
1035	Enhancement	Verified	Smokeview - change units display
1032	Enhancement	Verified	Particle flux in 2D CYLINDRICAL calcs
1031	Enhancement	Verified	Feature request: RAMP for particle mass flux
			FDS: Inaccurate air oxygen fraction causes error in fractional
	Defect	Verified	effective dose
1022	Defect	Verified	_hrr.csv energy balance
	Enhancement	Verified	User Guide: Fuel specific heat defaults
1010	Defect	Closed	Numerical Instability with 100 micrometer
1008	Defect	Invalid	Activation and deactivation of vents in dependence of

ID	Туре	Status	User Reported Summary [sic]
			temperature
1003	Defect	Accepted	pointer initialization
1001	Defect	Verified	ALLOCATABLE in TYPE Definitions Not Allowed in F95
999	Defect	Verified	aspiration_detector and FED verification cases broken
995	Defect	Verified	DEVC QUANTITY "RADIATIVE HEAT FLUX GAS" - wrong unit
982	Enhancement	Closed	Add premixed option to EDC
979	Defect	Verified	Incombustible wood
977	Defect	Invalid	Burner Position Results
976	Defect	Invalid	Mesh vents overlap and numerical instability
972	Enhancement	Accepted	Arbitrary species for toxicity computations
971	Enhancement	Closed	Implementation of Moinuddin and Li heat transfer model
969	Defect	AltInputs	FDS+Evac: 2 people stuck in 1.2m wide door!
965	Defect	WontFix	flame surface not steady state
964	Defect	Verified	installation error message
963	Defect	Verified	Volume fractions do not add up
962	Defect	Closed	Flame surface
958	Enhancement	Started	efficiency and conservation of boundedness correction
957	Defect	WontFix	flame surface out of domain
956	Defect	AltInputs	ERROR: Specify orientation of VENT 6, MESH 3
950	Defect	WontFix	heat and smoke detector problem
946	Defect	WontFix	Different HRR and fire behaviour with different versions of FDS
945	Defect	Verified	Dry oxygen
943	Defect	Verified	SPEC ID='WATER VAPOR'
942	Defect	Closed	Extinction criteria in fire.f90
			Changing Heat of Vaporization for water affects Relative
940	Defect	Verified	Humidity
			same file will run on fds 5.3.0 win 32 but won't run on fds 5.4.1
934	Defect	WontFix	win 2008 server 64 bit
932	Defect	Verified	Compilation Error in dump.f90 for Revision 5092
930	Defect	Invalid	&MISC U0 (Wind)
920	Defect	AltInputs	Memory allocation failed for PRHS in the routine INIT-FDS V5.4
919	Enhancement	Verified	modify unit string for DEVC
914	Defect	AltInputs	FDS Control Logic Error
910	Defect	Verified	Numerical instability with fire and sprinlers
-	Enhancement	OnHold	User defined, spatially dependent velocity profile at vent inlet??
	Defect	Verified	Negative gas enthalpy in part.f90
	Enhancement	Verified	drag law for cylinders
	Enhancement	WontFix	write ascii files from SMV, replaces fds2ascii
	Defect	Verified	SmokeView - Press G and Press C
-	Defect	Verified	Compile Error in divg.f90
	Defect	Verified	FDS6 transport scheme and extra species
-	Defect	Invalid	carbon monoxide production and modelling
	Defect	Duplicate	Issue similar to issue 633
	Defect	Closed	Path in osx 32bit mpi version is looking for /Users/gforney
859	Defect	Verified	incorrect guide reference to webpage

ID	Туре	Status	User Reported Summary [sic]
849	Enhancement	Verified	text contrast for grid labels
848	Defect	Invalid	Using FDS to simulate density stratification of gas mixtures
846	Other	WontFix	Getting error while compiling source code
844	Defect	AltInputs	Using Controls to Deactivate a Vent
838	Enhancement	OnHold	Feature Request - Control HRRPUA via DEVC or CTRL
			Energy conservation issue with fds5_linux and
835	Defect	Verified	fds5_intel_linux_64
			FDS Sprinkler - dissapearance of smoke and fire after sprinkler
831	Defect	Invalid	activation
			Backing='insulated' in input file conducting to 'exposed in the
830	Defect	Verified	output file
810	Defect	WontFix	Wrong Temperatures
807	Defect	Verified	Overhaul Helium and Hydrogen Validation Cases
800	Defect	Fixed	Different HRR before sprinkler activation
799	Defect	Invalid	SPEC in .out file
785	Defect	Fixed	Using beam detector over multiple meshes
777	Defect	Verified	Droplets do not stick on walls
774	Defect	MoreInfo	Sudden stop due to lock the hrr file and how to restart
773	Enhancement	WontFix	Plot logarithms of values in Smokeview
			Is CTRL and DEVC sharing among HOLEs and other objects now
	Defect	Verified	fixed?
	Defect	OnHold	FDS part.f90 - Total FRAC is greater than one
760	Defect	Verified	Clarification on Sprinkler Table Read
			simulated radiative flux drastically different from experimental
	Defect	WontFix	values
	Defect	Closed	droplets not dripping from ceiling
	Defect	Closed	No record of errors.
	Defect	WontFix	Execution error on newly downloaded version 5.3.1 of FDS
	Defect	WontFix	creation of velocity at boundaries for a steady flow at rest.
	Defect	Verified	FDS User Gude Error in section 6.2.1
	Defect	OnHold	Species vent error
	Defect	Verified	segfault with large number of SURF entries
	Defect	Verified	cp error with no additional species
	Defect	Verified	HRR for Q* cases too high with FDS6
	Defect	WontFix	FDS not picking up CHID or TITLE from HEAD line.
	Defect	AltInputs	RAMP function - any limit?
	Defect	Verified	CMP Section 3.1.2 SVN keyword expansion
	Defect	Verified	Warning message missing
	Defect	Verified	SVN 3255 and SVN 3263 produce significantly different results
	Defect	Verified	radiation_in_a_box verification case fails
	Enhancement	Verified	Enhancement: He specific heat
	Defect	Verified	"Typo" - CH4 shown as CH2
	Defect	OnHold	Adding OBST then adding HOLE does not work
	Defect	Verified	5.3.0 - DEADBAND Issue
664	Defect	Verified	2D cup burner crashes

ID	Туре	Status	User Reported Summary [sic]
657	Defect	Verified	Suspicious difference in density measurement
			FDS has overpredicted a heat loss of 2 times for fluid travelling
655	Defect	WontFix	along a long duct or a tunnel
			DROPLETS_PER_SECOND default inconsistent with
654	Defect	Verified	documentation
653	Defect	Closed	DROPLET and PARTICLE_CLASS, TARGETS and POINTERS
649	Defect	AltInputs	The problem of FDS when using MPICH2
639	Defect	Duplicate	Temperature behaviour
636	Defect	Verified	Sprinkler
			FDS Test Case: water_evaporation not following description in
630	Defect	Fixed	User Guide
628	Defect	Verified	dynsmag and mass error
617	Defect	WontFix	Visualization issue
614	Defect	Verified	FDS User Guide: Sample files no longer included in installation
606	Defect	Verified	OBSTs disapper although PERMIT_HOLE is used
599	Defect	Verified	FDS - Pointer not associated with a target error
			Vents are rejected because boundary already has mateiral
598	Defect	AltInputs	property vent
595	Defect	UnVerified	can not run fds5_mpi.exe
594	Enhancement	OnHold	POROUS SURFACES
593	Defect	Duplicate	Porous surfaces
592	Defect	Verified	Picture rendering in SMV defect
590	Defect	Verified	CP_TMP array subscript error
589	Defect	Verified	SPEC_ID='MIXTURE_FRACTION_1' not working
588	Defect	Verified	smv 2866 dies loading slice
			Access violation error on 5.2.5 only (5.2.4 OK). Flush buffers
585	Defect	Verified	doesn't help.
584	Defect	Verified	SPRINKLER ORIENTATION
581	Defect	Verified	Smokeview display of detector activation
580	Defect	WontFix	Problem viewing sprinkler particles
572	Defect	WontFix	errno64
	Defect	Duplicate	temperature at the edge of the burner
	Defect	AltInputs	Control Function
	Enhancement	WontFix	Replace INERT with COLDWALL?
	Defect	Verified	Single DEVC with PROP_ID
555	Defect	AltInputs	Help with MESH out of alignment
	Defect	Verified	post_processing_linux_cluster
	Defect	Verified	Describe how mutli layer surfaces are applied to OBST in U Guide
	Defect	Verified	Smokeview Documentation of Setting Manual Frame Skip
	Other	Verified	Periodic breaks in usage of processor
	Defect	Verified	Users Guide Clarification on Ramp Behaviour
-	Defect	Verified	Output quantity: specific heat
	Defect	Verified	Explanation of STATISTICS in Users Guide
-	Enhancement	Verified	Add net heat flux BC
520	Defect	Verified	State file problem

ID	Туре	Status	User Reported Summary [sic]
519	Defect	Started	HRR and CONV_LOSS not matching
515	Defect	Invalid	&DEVC for soot density usin FDS 5.2.2
512	Defect	WontFix	Problem about POROUS OBST
509	Defect	Verified	POROUS OBST
508	Defect	AltInputs	SURF causing display error
507	Defect	WontFix	Ghost fire !
505	Defect	Verified	Smoke leakage through OBSTs
504	Defect	Verified	TRN feature
501	Defect	Verified	Computation of specific heat in divg.f90
497	Defect	OnHold	Control and removing of obstructions
494	Defect	WontFix	Controlling vents with aspiration smoke detectors
486	Defect	Verified	using CTRL function to ramp down fan
485	Defect	UnVerified	Sprinkler Flow Problem
483	Defect	Verified	reactions stop immediately and furniture disappear
479	Defect	Verified	Check output quantity table
475	Defect	Verified	Exchange of MU in Multi-Mesh calculations
469	Defect	Verified	Too much HRR in finite rate calc.
466	Defect	Verified	Wrong Types in EVAC routine
465	Other	Verified	U-Guide DEVC_DUMP_LIMIT
461	Defect	WontFix	hrr.csv result values while using adiabatic walls
459	Defect	Verified	CO Production Measurement
439	Defect	Verified	Explanation of "IDEAL" in Users Guide
437	Defect	AltInputs	Flow problem between meshes
427	Defect	OnHold	Problem with function BLACKBODY_FRACTION
409	Defect	WontFix	getting high HRR and low CO
			BOUNDARY_DEFAULT feature does not work for default
408	Defect	Verified	boundaries defined by FDS
	Defect	Verified	VnV csv file and Excel comma padding
	Defect	Verified	Error in reaction product formula
375	Defect	Verified	Entry misspelled in index
360	Defect	WontFix	Water vapor pressure
			Summarize the input production of additional species, and its
	Defect	WontFix	balance.
	Defect	Verified	Output of "OTHER"
	Enhancement	Verified	pyrolysis model - combustion fuel gases
	Defect	AltInputs	Insufficient memory allocation and bus error
	Defect	WontFix	FDS5 vs FDS4 Performance
	Defect	Verified	VENT will not work for time < 0
	Defect	Verified	DEVC XB input read limit set too small
	Defect	Verified	Numerical Instability and Sprinkler
	Defect	Verified	Access Violation
	Defect	Verified	'Spread-rate' function dows not wok with VENT control logic
	Defect	Verified	Problem on aspiration detection modelling
	Defect	UnVerified	Segmentation Fault on Intel MacPro
198	Enhancement	WontFix	DEVC output for leakage flows

ID	Туре	Status	User Reported Summary [sic]
186	Defect	Verified	FDS fails when trying to write to a READONLY file
161	Defect	Verified	Optical density
116	Defect	Fixed	Composition of incoming supply "air"
76	Defect	WontFix	RESTART feature
21	Enhancement	Verified	Enhancements wish list - low priority

## **APPENDIX D: Discussion Forum**

Below is a summary of the author's participation in the FDS online forum during the 2008-2011 reporting period (624 posts to the forum).

Month	Number of Postings
September, 2008	7
October, 2008	13
November, 2008	35
December, 2008	22
January, 2009	33
February, 2009	30
March, 2009	27
April, 2009	13
May, 2009	17
June, 2009	21
July, 2009	20
August, 2009	24
Yearly Total	262
September, 2009	36
October, 2009	23
November, 2009	15
December, 2009	20
January, 2010	13
February, 2010	18
March, 2010	16
April, 2010	19
May, 2010	20
June, 2010	12
July, 2010	13
August, 2010	15
Yearly Total	220
September, 2010	8
October, 2010	11
November, 2010	12
December, 2010	6
January, 2011	9
February, 2011	8
March, 2011	11
April, 2011	8
May, 2011	13
June, 2011	17
July, 2011	23
August, 2011	16
Yearly Total	142
	142