

The State of Art model Fire Dynamics Simulator: Feasibility of Introduction of New RAMP and Tabular Functions.

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Abstract

Fire Dynamics Simulation (FDS) is commonly used computational fluid dynamics (CFD) based fire model in research and practical engineering applications. Various thermo-physical material properties and chemical kinetics values are needed as the input parameters. To account for variation of some of the property values with respect to temperature; RAMP and tabular functions are used. This paper identifies additional properties whose variation in heating rate and radiation flux can be implemented using new RAMP and tabular functions.

Introduction

Performance-based design has now become the method/approach preferred by fire engineers and researchers. This is driven by the flexibility offered to the user to adopt their new design concept without compromising safety aspects required by regulation. As an experimental study is vastly expensive, numerical simulation is an alternative method to test fire safety system/design.

FDS is a state of the art CFD based fire model developed by the National Institute of Standards and Technology (NIST). This programme is widely used to simulate practical fire scenarios and also as a research tool to study fire dynamics and combustion [1]. It was first released in February 2000; since then it has continuously growing and improving with collaboration and contribution from private organisations and also users among this community.

The FDS is designed to model a number of fire phenomena including pyrolysis. Like any other numerical model, various input parameters are required for FDS. These include thermal material properties and chemical kinetics of the studied material; a number of them are constant while others are varied in respect to temperature, heating rate, etc. In fire situations, the temperature of materials (both combustible and non-combustible) and incident radiation constantly change. The FDS handles the change of some material property values with respect to material temperature using thermal RAMP and tabular functions. In this paper the possibility of extending these functions in FDS for wider parameters is discussed.

Existing RAMP Function for Thermal Properties

Thermal material properties (such as specific heat, C_p and thermal conductivity, k) define fire behaviour of a material and also a key component in predicting/understanding fire growth and development. Experimental data presented in Fig 1 shows that these two parameters of a material vary with material's temperature, almost linearly. Currently, with the RAMP function of these thermal properties can be specified as functions of temperature.

The RAMP function allows users to control the behaviour of these two parameters as found experimentally. The behaviour can be linear or non-linear. An example of the RAMP function is given below:

```
&MATL ID = 'STEEL'  
  FYI = 'A242 Steel'  
  SPECIFIC_HEAT_RAMP = 'c_steel'  
  CONDUCTIVITY_RAMP = 'k_steel'
```

```

DENSITY = 7850. /
&RAMP ID='c_steel', T= 20., F=0.45 /
&RAMP ID='c_steel', T=377., F=0.60 /
&RAMP ID='c_steel', T=677., F=0.85 /

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

```

It is to be noted that for values of temperature, T , (1) below and above the given range, FDS will assume a constant value equal to the first or last F specified and (2) between two consecutive T values, parameter values increase/ decrease linearly. With this setting, the fire growth and development is being simulated by using a set of property values at various temperatures.

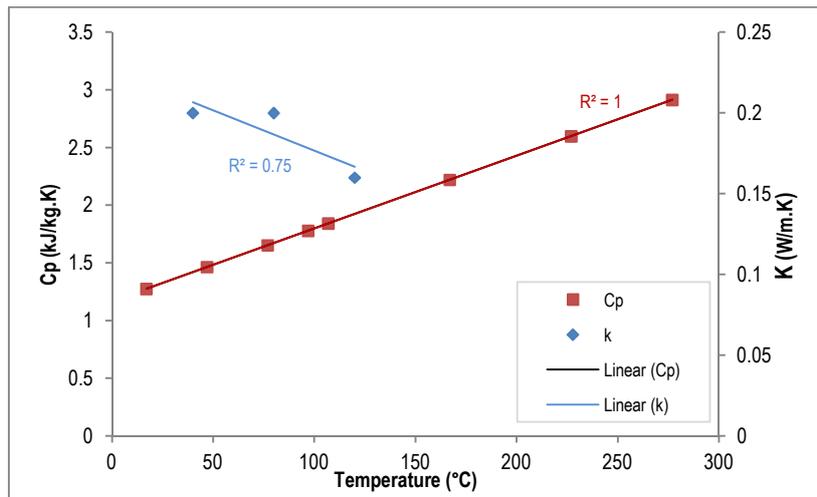


Figure 1: Material properties of PMMA change with respect to temperature: C_p from [2], k from [3]

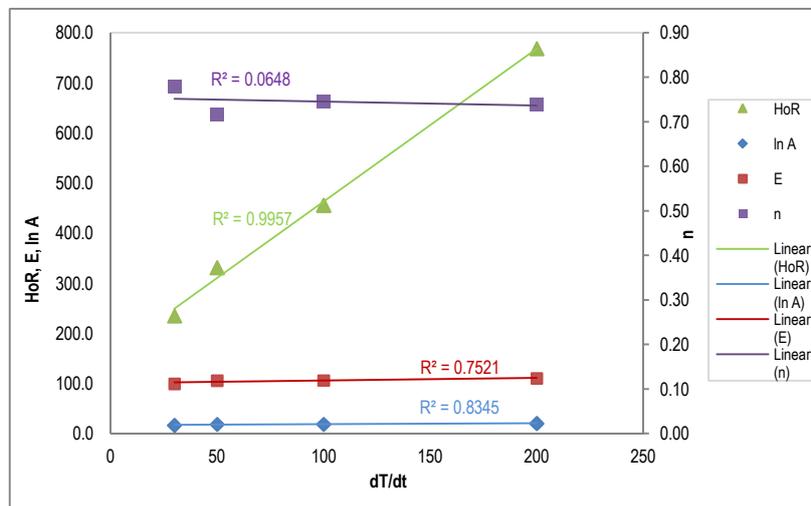
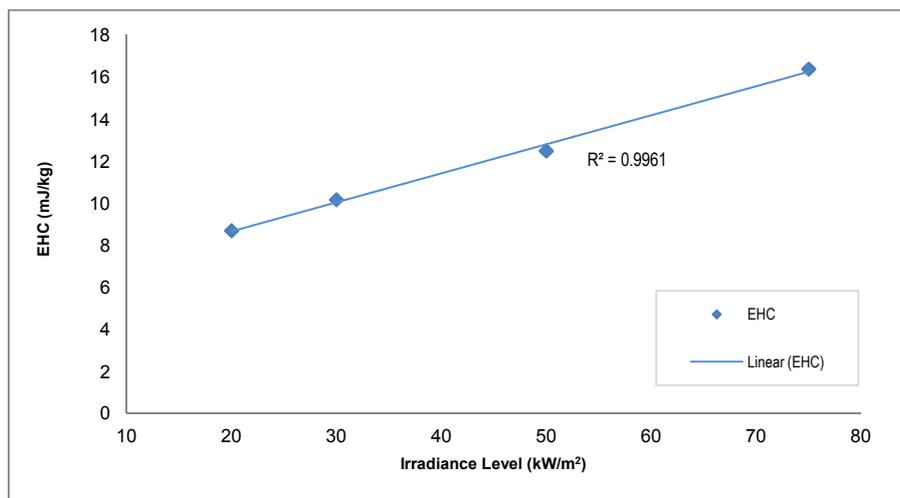


Figure 2: Chemical kinetics and material properties change with respect to dT/dt (pinewood).

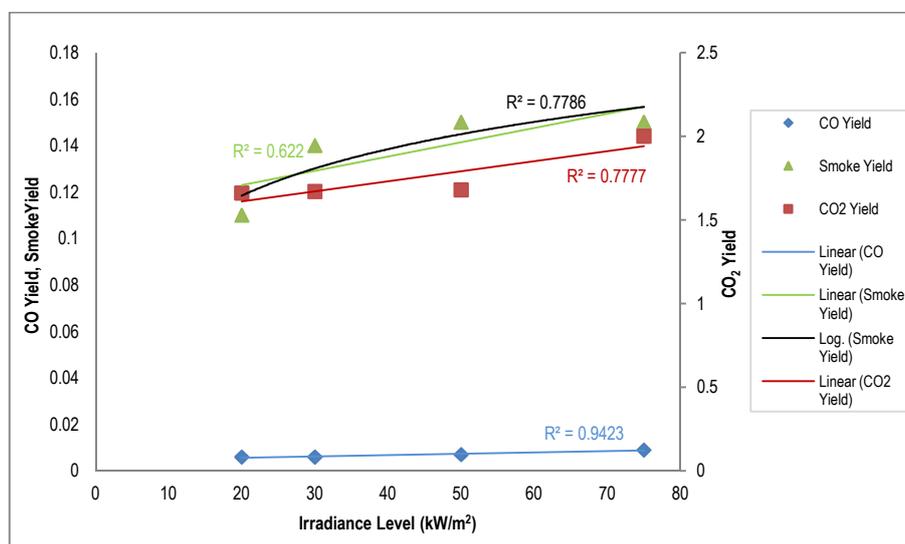
Proposed RAMP Function for Chemical Kinetics

In a real fire event, as the fire grows, the combustible materials exposed to fire are heated up at different heating rates (dT/dt). Kinetic parameters (activation energy, E , reaction order, n , and pre-exponential factor, A) and Heat of Reaction (HoR) vary with the heating rates. It can be observed in Fig 2 that parameter values of A , E , n and HoR vary with dT/dt for pinewood.

Ideally simulation should be performed by using the appropriate value as per fire condition representing the current heating rate at each point. Currently FDS has no provision of specifying the dT/dt dependent values of parameters. However, similar to the temperature RAMP function described above, heating rate RAMP functions (ACTIVATION_ENERGY_RAMP, HEAT_OF_REACTION_RAMP, PREEXPONENTIAL_FACTOR_RAMP and REACTION_ORDER_RAMP) can be used in FDS. As the heating rate increases or decreases, the RAMP function will play its role by providing appropriate material properties value representing the actual condition. This will enable the simulation to provide more accurate results according to a fire condition. As FDS calculates the temperature history of each solid cell, it is possible to calculate dT/dt for every time-step. For simplicity, FDS may need to use parameter values of the previous time-step for the current time-step.



(a) Effective heat of combustion



(b) CO yield, CO₂ yield and smoke yield

Figure 3 Parameters obtained from the cone calorimeter for PMMA,

It is to be noted that in the current version of FDS (version 5) [1], sets of kinetics (A , E and n) are used to describe multi-step reactions corresponding to the components of the combustible, like hemicelluloses, cellulose and lignin in wooden materials. FDS developers suggested methods for determining the kinetics for each component using bench-scale measurement techniques. With the suggestion of using RAMP functions relevant to the heating rate, it will be interesting to assess

whether the kinetics under various heating rates rather than the kinetics of the components is more critical in modelling of pyrolysis and combustion or much complicated, the proposed function of heating rate should be applied to the kinetics of the individual reaction. It's suggested that the FDS research community to conduct an assessment (verification and validation) of impacts on pyrolysis and combustion from applying those various algorithms of kinetics parameters.

Variation of parameter values of Effective Heat of Combustion (EHC), CO yield, CO₂ yield and smoke yield with respect to change of radiative heat flux can be measured using a cone calorimeter. Figure 3 shows these variations, for example EHC increases as heat flux is increased. As FDS calculates radiative heat flux on each solid surface, it is possible to introduce an IRRADIANCE_RAMP function for every time-step.

It is to be noted that various gas and soot yields values are averaged from normal measurements in the cone calorimeter over a certain length of testing time with constant irradiation levels [4]. However, it has been observed that those parameters vary during the tests even under constant irradiation from the heating element in cone calorimeter. This is even true when charring materials are involved since presenting of char and its thickness have various influences on the gas and soot generations. It may argue that more complicated algorithm needs to develop to reflect the changes of values with respect to irradiance, time, material thickness, char fraction etc. However, the proposed method in relation to Fig 3, can be considered as the first step towards better use of the bench scale data. It is expected that in future more advanced algorithm will be developed in relation to gas and soot yields.

Existing Tabular Function

To account for multi-dimensional variation of input quantities, FDS uses the TABL function. Currently it is only used for prescribing sprinkler spray pattern via SPRAY_PATTERN_TABLE command. An example is given below:

```
&PROP ID='K-11',  
    QUANTITY='SPRINKLER LINK TEMPERATURE',  
    OFFSET=0.10,  
    PART_ID='water_drops',  
    FLOW_RATE=60.,  
    SPRAY_PATTERN_TABLE='TABLE1',  
    SMOKEVIEW_ID='sprinkler_upright',  
    DROPLET_VELOCITY=10. /
```

```
&TABL ID='TABLE1', TABLE_DATA=independent parameter1 set1, independent parameter2 set2,  
dependent parameter1, dependent parameter2/
```

```
&TABL ID='TABLE1', TABLE_DATA=independent parameter1 set2, independent parameter2 set2,  
dependent parameter1, dependent parameter2/
```

Here two dependent variables (droplet velocity and a fraction of the volume flow rate) vary with two sets of independent variables (bound of latitude and bound of longitude). In the next section two new tabular functions are proposed, where multiple dependent variables vary with one independent variable.

Proposed Tabular Function for Thermal Properties and Kinetics

It has been observed in [5] that the specific heat- temperature profiles vary with the heating rate as shown in Fig 4. This phenomenon is unlikely to be modelled by SPECIFIC_HEAT_RAMP function only. However as the single variable is dependent two relatively independent variables T and dT/dt , it is possible for FDS developers to develop a new tabular function SPECIFIC_HEAT_TABLE function. An example is given below:

&TABL ID='TABLE1', TABLE_DATA= HEATING_RATE1, TEMP_S1, TEMP_E1, SPECIFIC_HEAT_M1/
 &TABL ID='TABLE1', TABLE_DATA= HEATING_RATE2, TEMP_S2, TEMP_E2, SPECIFIC_HEAT_M2/

TEMP_S, TEMP_E and SPECIFIC_HEAT_M represent starting temperature, T_s , ending temperature, T_e and peak value at ending temperature, $C_{p,max}$, respectively. For any material temperature, T_i , between the starting and ending temperatures at a specific heating rate, the specific heat capacity, $C_{p,i}$ can be calculated as:

$$C_{p,i} = C_{p,max} \times \frac{T_i - T_s}{T_e - T_s} \dots\dots (1)$$

For a heating rate not listed in the table, its T_s , T_e and $C_{p,max}$ can be chosen as average values of the previous and the next heating rate. However, below and above the given range of the heating rate, constant values equal to the first or last set of heating rates to be assumed.

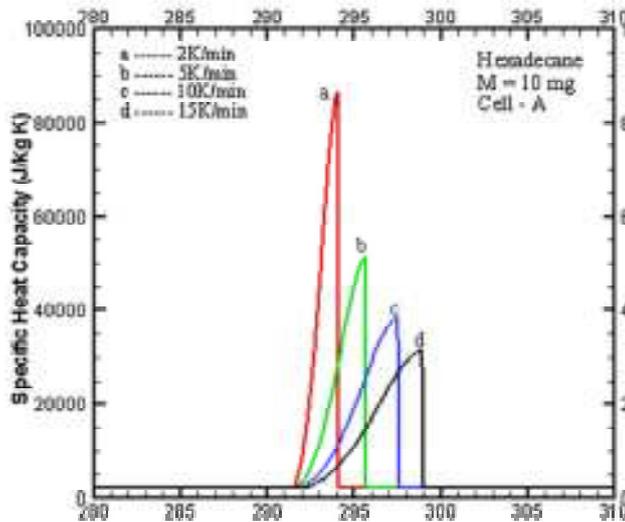


Figure 4: Effect of the heating rate on the specific heat –temperature profiles.

It has been observed in [2] that parameter values of A , E and n of some combustible materials (such as PMMA) don't vary in any specific pattern. When FDS simulations of a cone calorimeter test configuration (without flaming combustion) at 25kW/m^2 irradiation are carried out with various sets of kinetic parameters (obtained at various heating rates) a specific pattern is observed. It is illustrated in Fig 5 where the mass loss rate (MLR) increases when the set of kinetic parameters obtained at higher dT/dt is used.

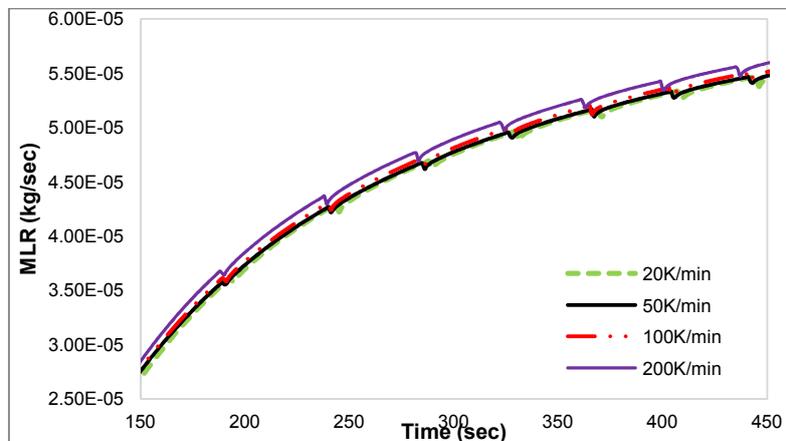


Figure 5: Effect of heating rates on kinetics parameters (PMMA)

It is recommended another TABL function be developed, so that all three parameters are within a KINETIC_TABLE function as given below:

```
&TABL ID='TABLE1', TABLE_DATA=HEATING_RATE1, ACTIVATION_ENERGY1,  
PREEXPONENTIAL_FACTOR1, REACTION_ORDER1/  
&TABL ID='TABLE1', TABLE_DATA=HEATING_RATE2, ACTIVATION_ENERGY2,  
PREEXPONENTIAL_FACTOR2, REACTION_ORDER2/
```

Here, for simplicity, instead of linear variation between two consecutive TABLE ID lines, a midpoint threshold can be used. However, below and above the given range, constant values equal to the first or last set of specified values to be assumed.

Conclusion

FDS provides output parameters such as gas and solid temperatures, radiation flux, CO, CO₂, smoke and other toxic gas concentrations. These parameters are largely dependent on the input data of thermo-physical properties and reaction parameters of combustible materials in building. More accurate application of input parameters is likely to improve the prediction of output parameters such as toxic gases released from combustible materials and radiant heat and temperature exposure which can be a major threat to human life. The approaches proposed in this paper are expected to make an improvement of the FDS fire model resulting in increased reliability in prediction of fire behaviour.

References

- [1] McGrattan, K.B., Hostikka, S., Floyd, J., Baum, H. & Rehm, R. 2008, *Fire Dynamics Simulator - Technical Guide, Version 5 Edn*, National Institute of Standards and Technology, Gaithersburg, MD USA.
- [2] Abu-Bakar, A. and Moinuddin K. 2012, Effects of variation in heating rate, sample mass and nitrogen flow on chemical kinetics for pyrolysis, *18th Australasian Fluid Mechanics Conference* December 3-7, Launceston, Australia.
- [3] Steinhaus, T. 1999, *Evaluation of the Thermophysical Properties of Poly (Methylmethacrylate) : A Reference Material for Development of A Flammability Test for Micro-Gravity Environments*, University of Maryland.
- [4] AS/NZS 3837 Cone Calorimeter standards (ISO 5660–1 ASTM E 1354)
- [5] Kousksoua, T., Jamilb, A., El Omari, K., Zeraouli, Y. And Le Guer, Y. 2011, Effect of heating rate and sample geometry on the apparent specific heat capacity: DSC applications *Thermochimica Acta* 519, 59-64.