UNIVERSITY OF CHEMISTRY AND TECHNOLOGY PRAGUE
Faculty of Chemical Engineering
Department of Chemical Engineering

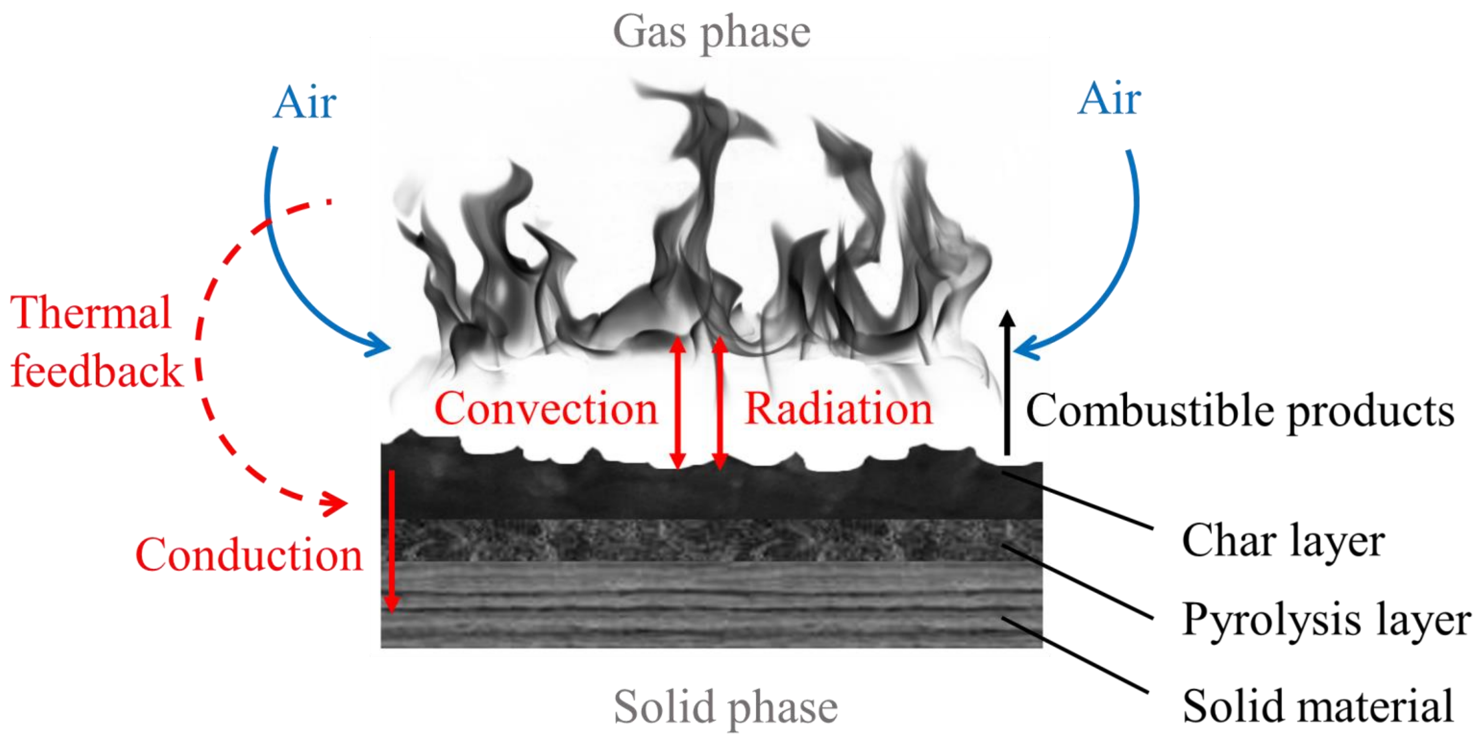
Advanced Pyrolysis Model Approach in FDS

Author: ***M.Sc. Vojtěch Šálek***

Supervisor: *Assoc. Prof. Milan Jahoda*

Supervisor-specialist: *Dr. Lucie Hasalová*

Pyrolysis

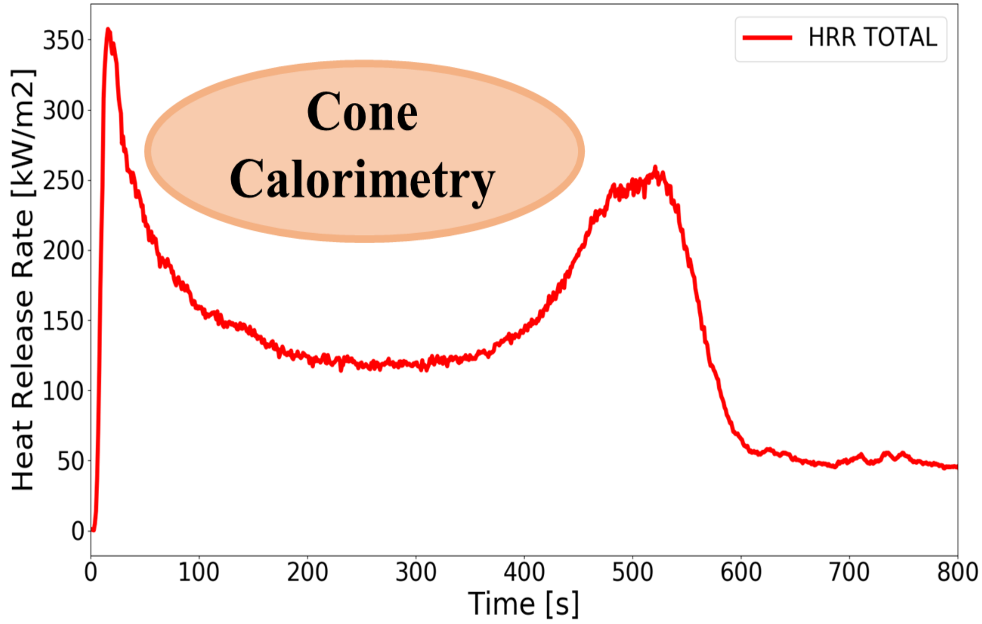


- Gaseous phase influence solid phase and vice versa
- How fast is gasification? $\dot{m}$ (mass loss rate, MLR)
- FDS (Fire Dynamics Simulator)
- Different approaches (variously complex), **2** main

Fire Consequence Modeling

- HRR (Heat release rate) - $\dot{q}''$
- Heat of combustion - ΔH_C

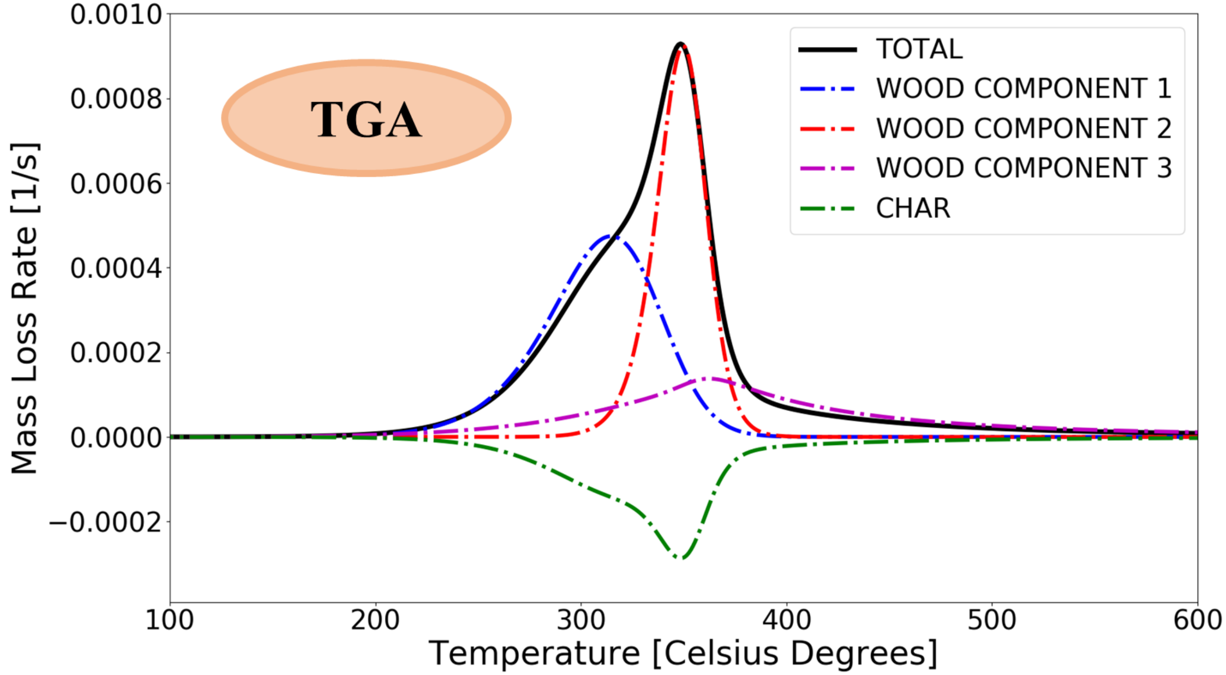
$$\dot{q}'' = \dot{m}\Delta H_C$$



ANAMET. Fire Testing Technology Ltd. http://www.anamet.cz/vyrobce/fire-testing-technology-ltd (cited 26.11.2019).

Complex Pyrolysis Modeling

- Heat transfer, heat conduction, decomposition kinetics, combustion, smoke production and transport, etc.
  -> complicated – a lot of input parameters
- Both gas and solid phase solved at the same time



$$\nu_1 \, Wood\ component\ 1 \longrightarrow \nu_{CH,1}\ Char + Combustible\ gases$$
$$\nu_2 \, Wood\ component\ 2 \longrightarrow \nu_{CH,2}\ Char + Combustible\ gases$$
$$\nu_3 \, Wood\ component\ 3 \longrightarrow \nu_{CH,3}\ Char + Combustible\ gases$$

Consequence vs. Complex Modeling

Consequence modeling parameters
Pyr. gas composition
Soot yield
Density
Heat conductivity
Specific heat
Emissivity
Heat release rate
Ignition temperature

11 vs. **30**

Complex modeling parameters	***How to obtain***
Pyr. gas composition	El. analysis, lit.
Soot yield	Cone calorimetry
Density	Directly, lit.
Heat conductivity	Exp., literature
Specific heat	DSC, literature
Emissivity	Literature
Char density	Directly, lit.
Char heat cond.	Exp., literature
Char specific heat	DSC, literature
Char emissivity	Literature
Preexp. factor	TGA – opt.
Activation energy	TGA – opt.
Order of reaction	TGA – opt.
Heat of reaction	DSC
Heat of combustion	Cone calorimetry
Stoch. coeff. of char	TGA
Stoch. coeff. of decomposing comp.	TGA – opt.

- Is 11 enough? For which scenario?
- Validation!

RCT (Room Corner Test)

- Test facility to determine Reaction to fire of facing materials (walls and ceilings)
- Burner location and fire load according to ISO 9705-1
- Room 2,4 x 3,6 x 2,4 m + hood 3 x 3 m + exhaust duct
- Walls covered by OSB board

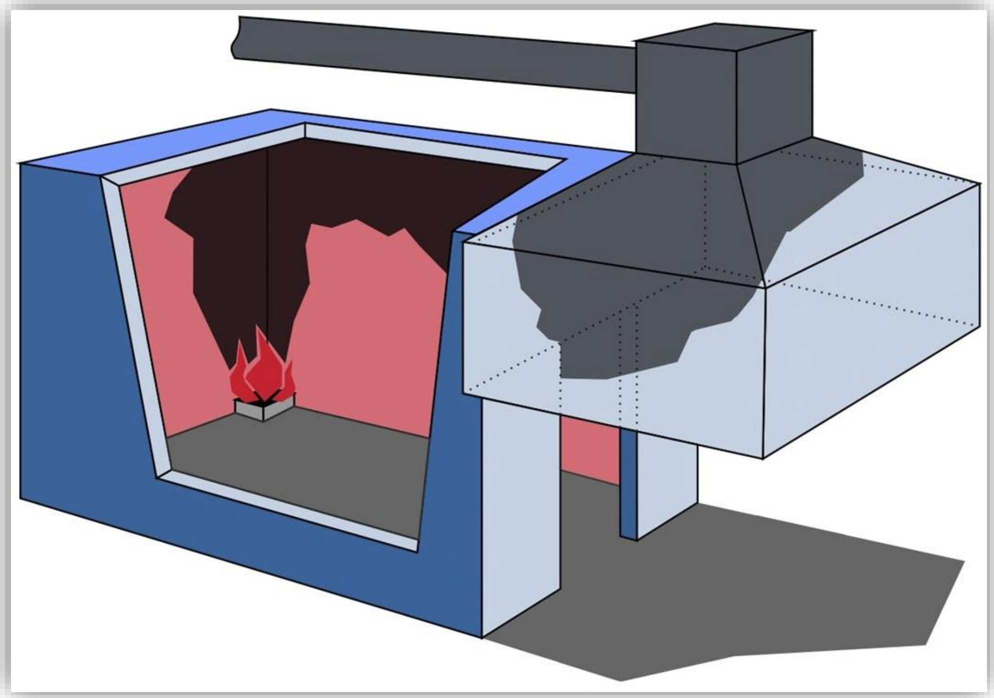
INTERNATIONAL STANDARD

ISO 9705-1

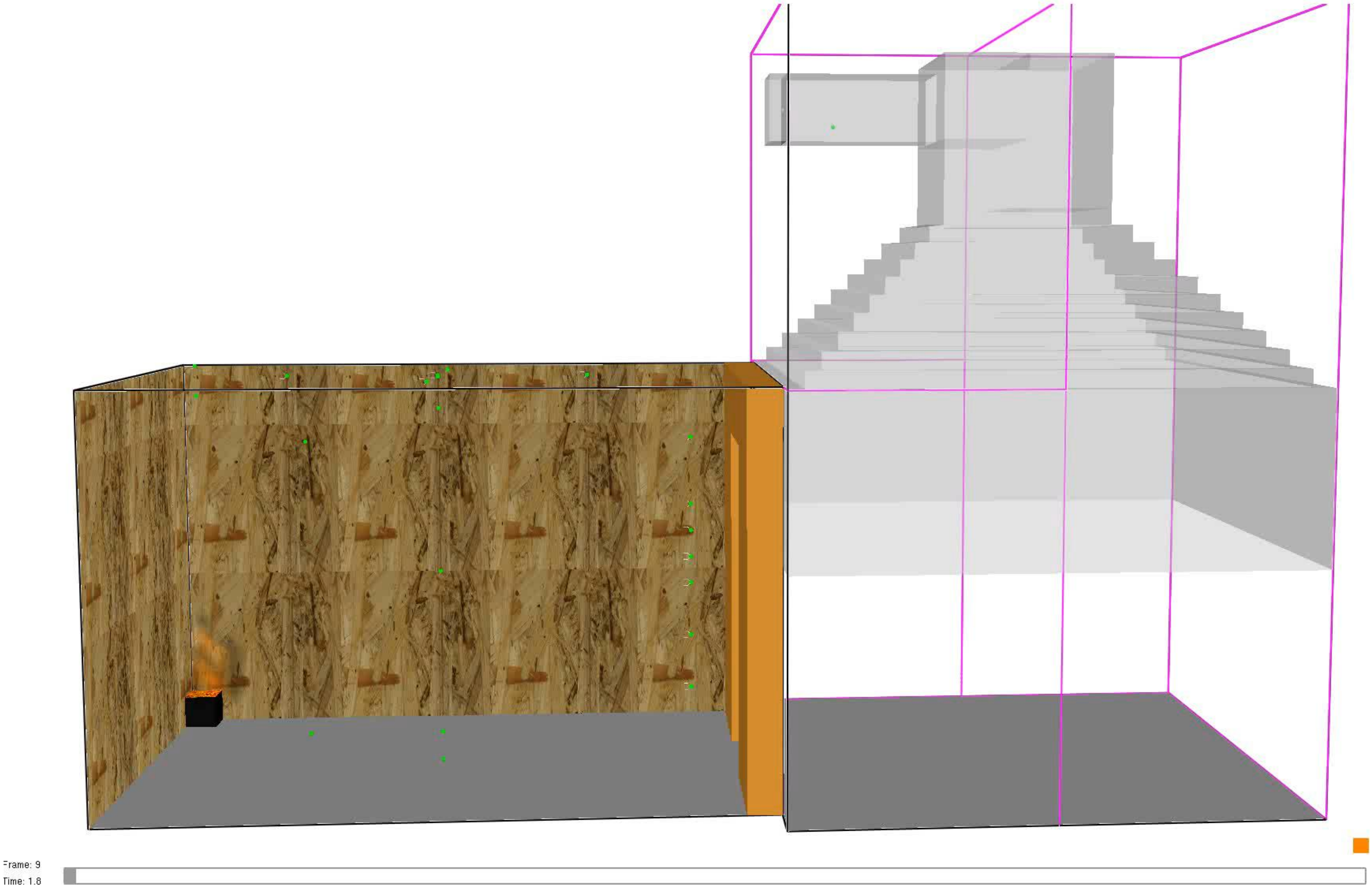
First edition
2016-02-15

Reaction to fire tests — Room corner test for wall and ceiling lining products —

Part 1:
Test method for a small room configuration



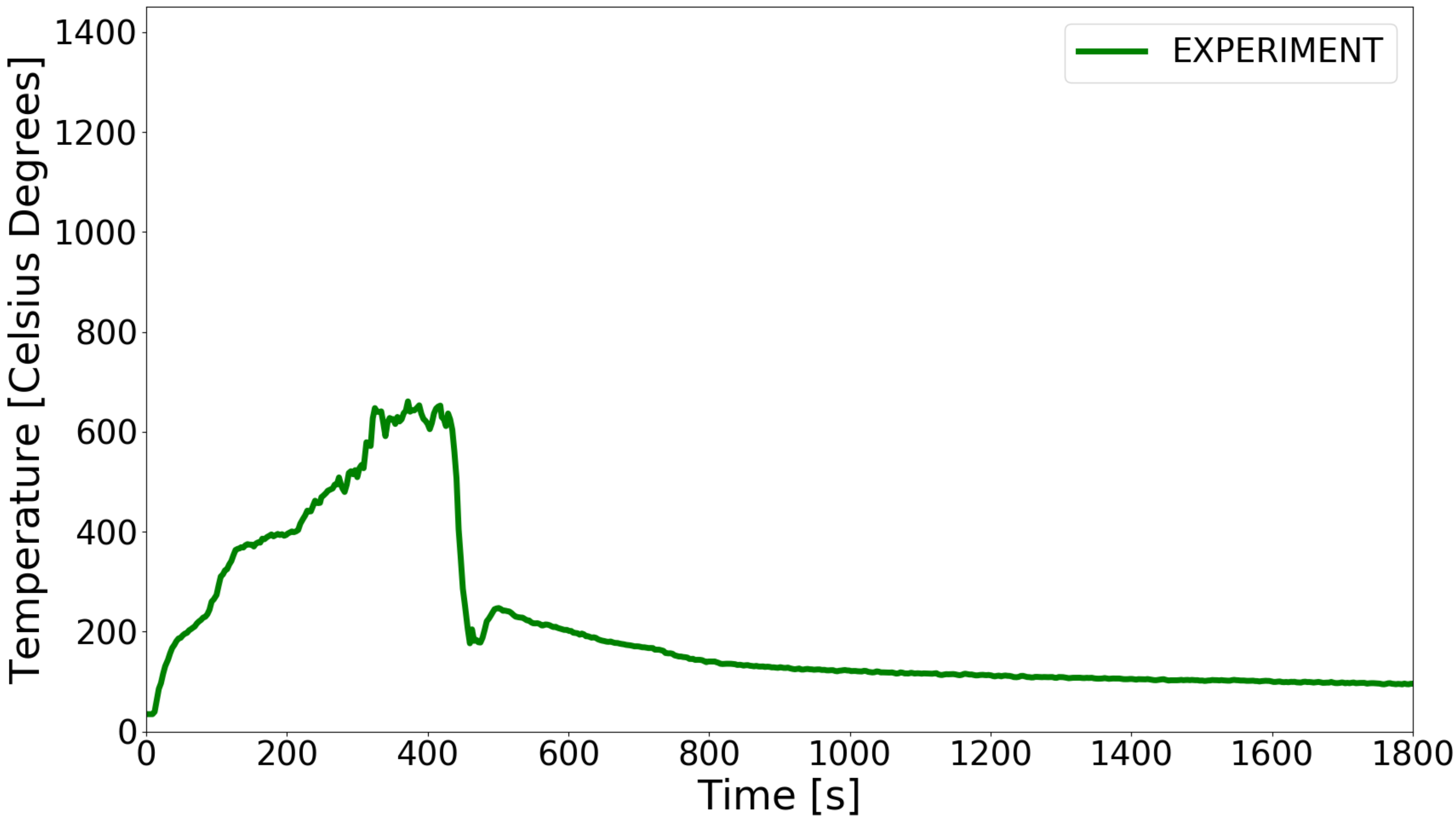
Room Corner Test – FDS model



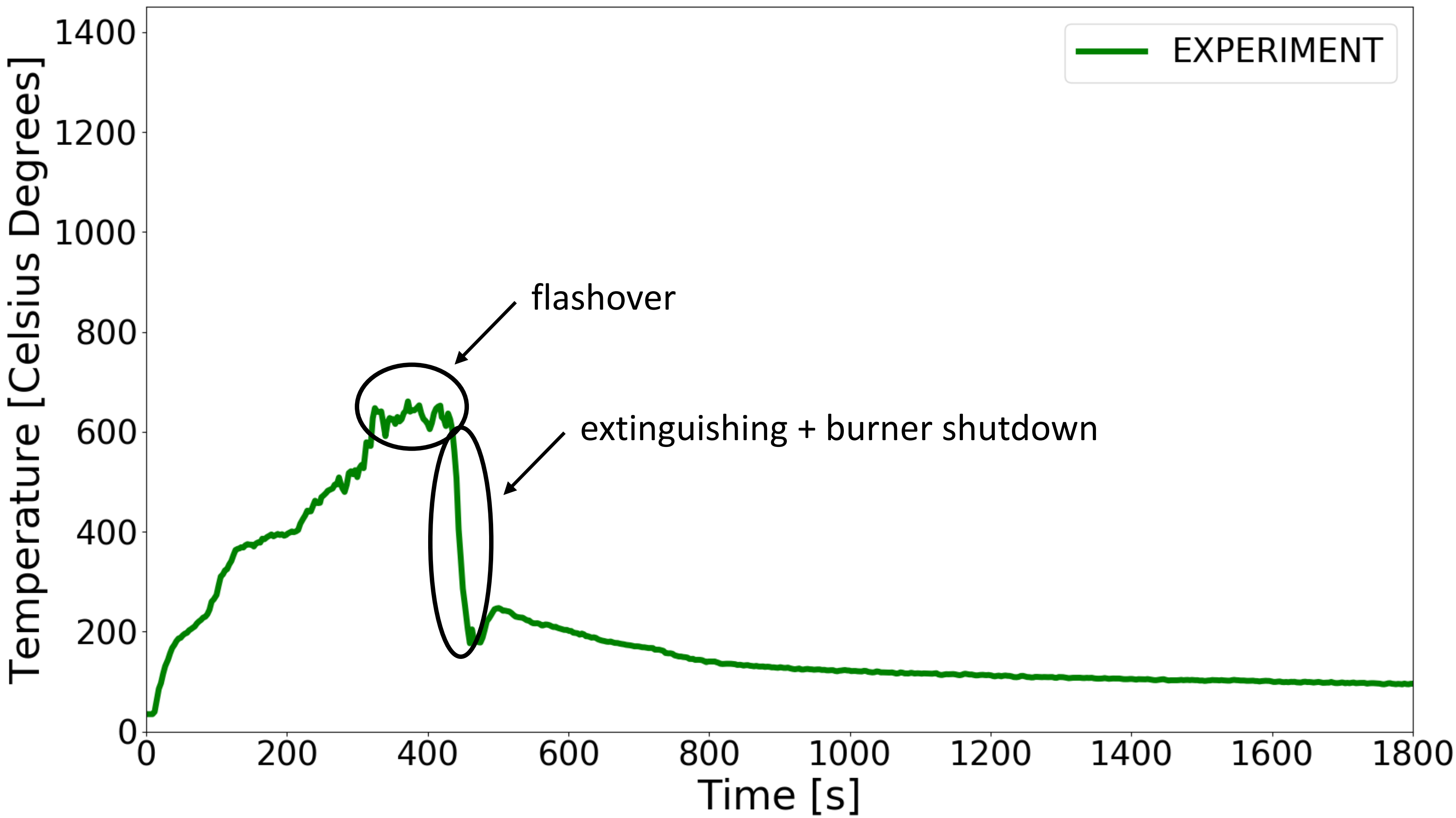
Investigated Material - OSB

- Engineered/Composite board
- Building material, insulation, interiors
- Charring, inhomogeneous
- Complex chemical structure (lignin, cellulose, hemicellulose) + adhesives + additives

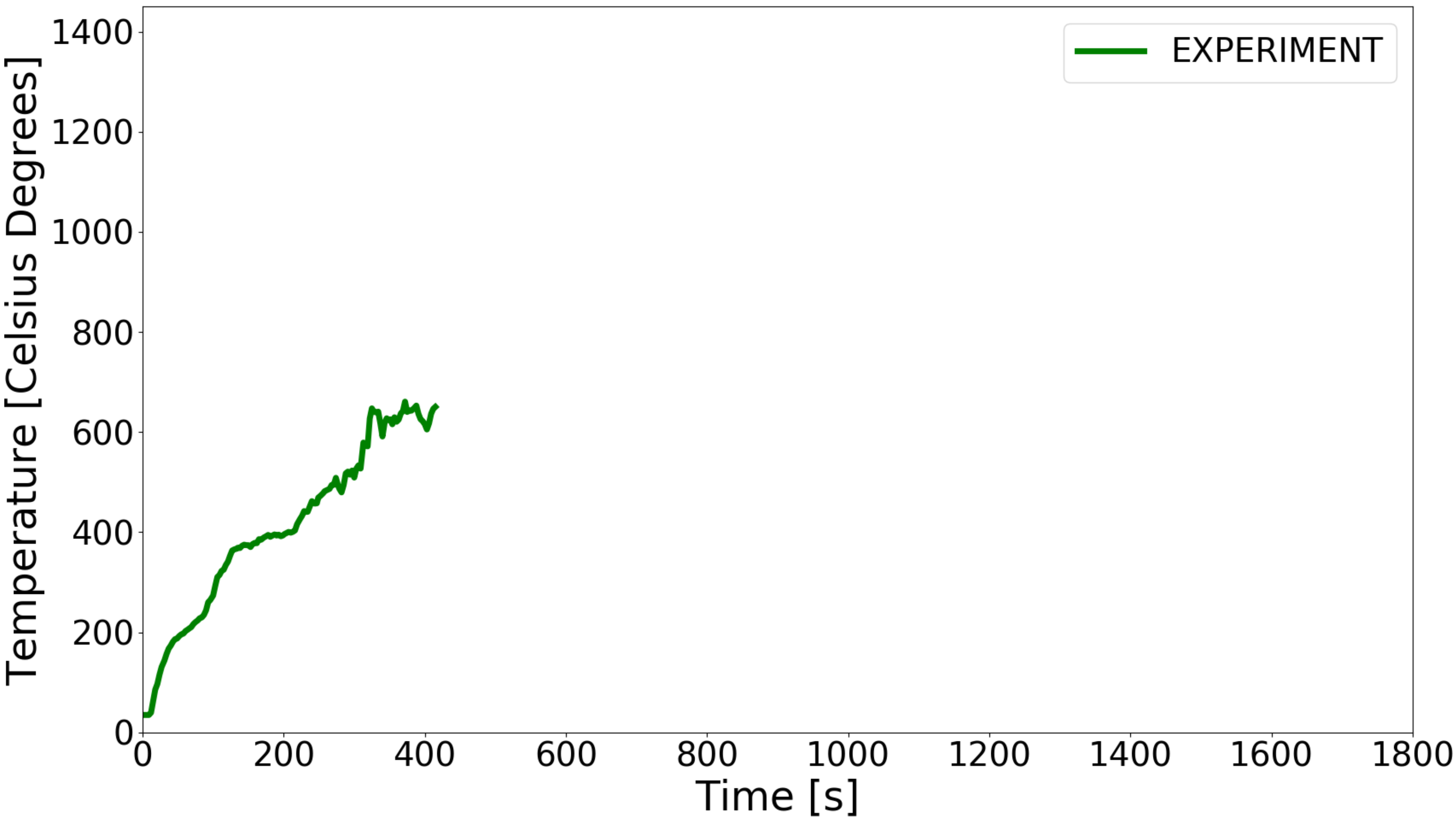
Experimental Data - Thermocouple



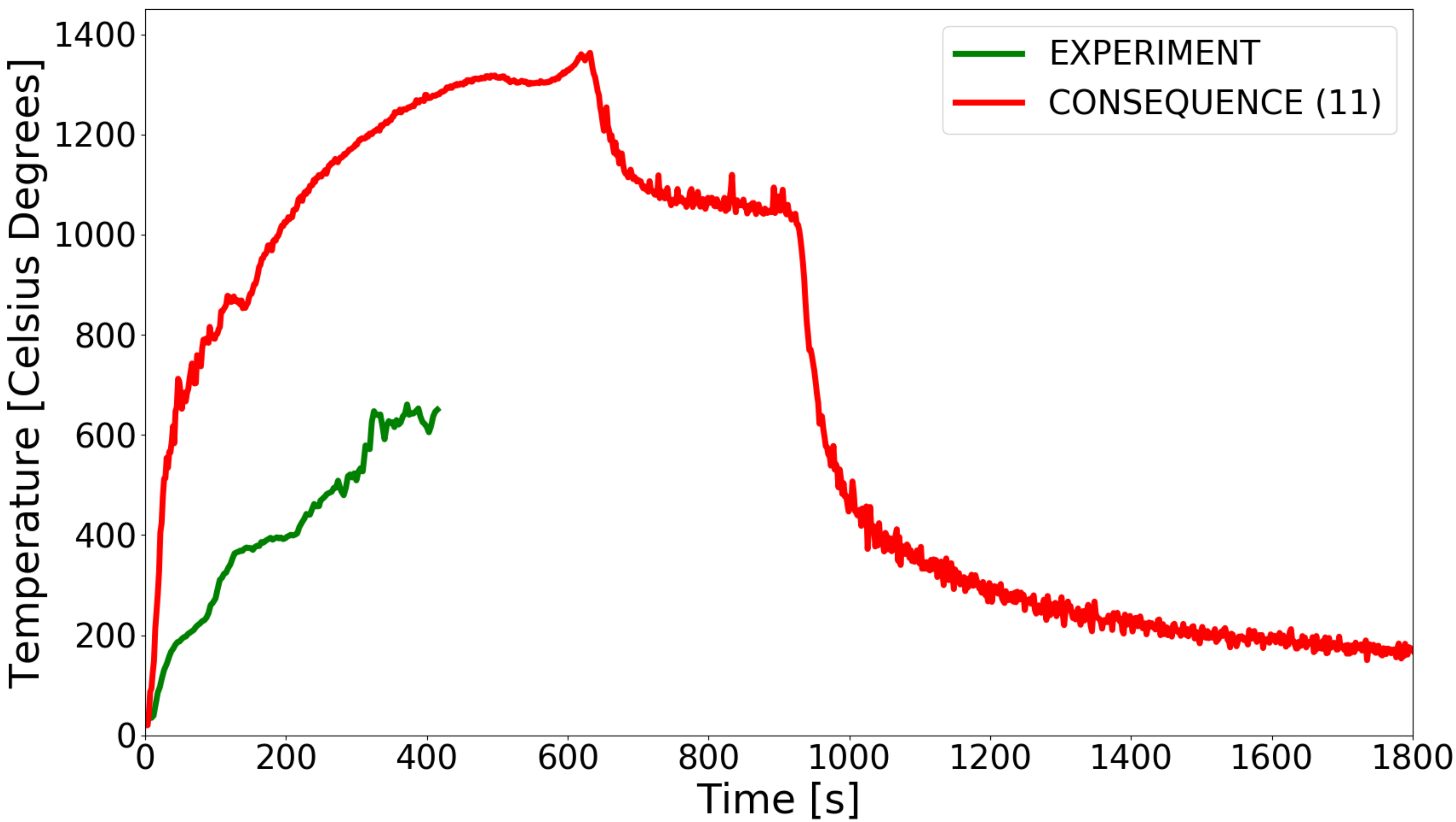
Experimental Data - Thermocouple



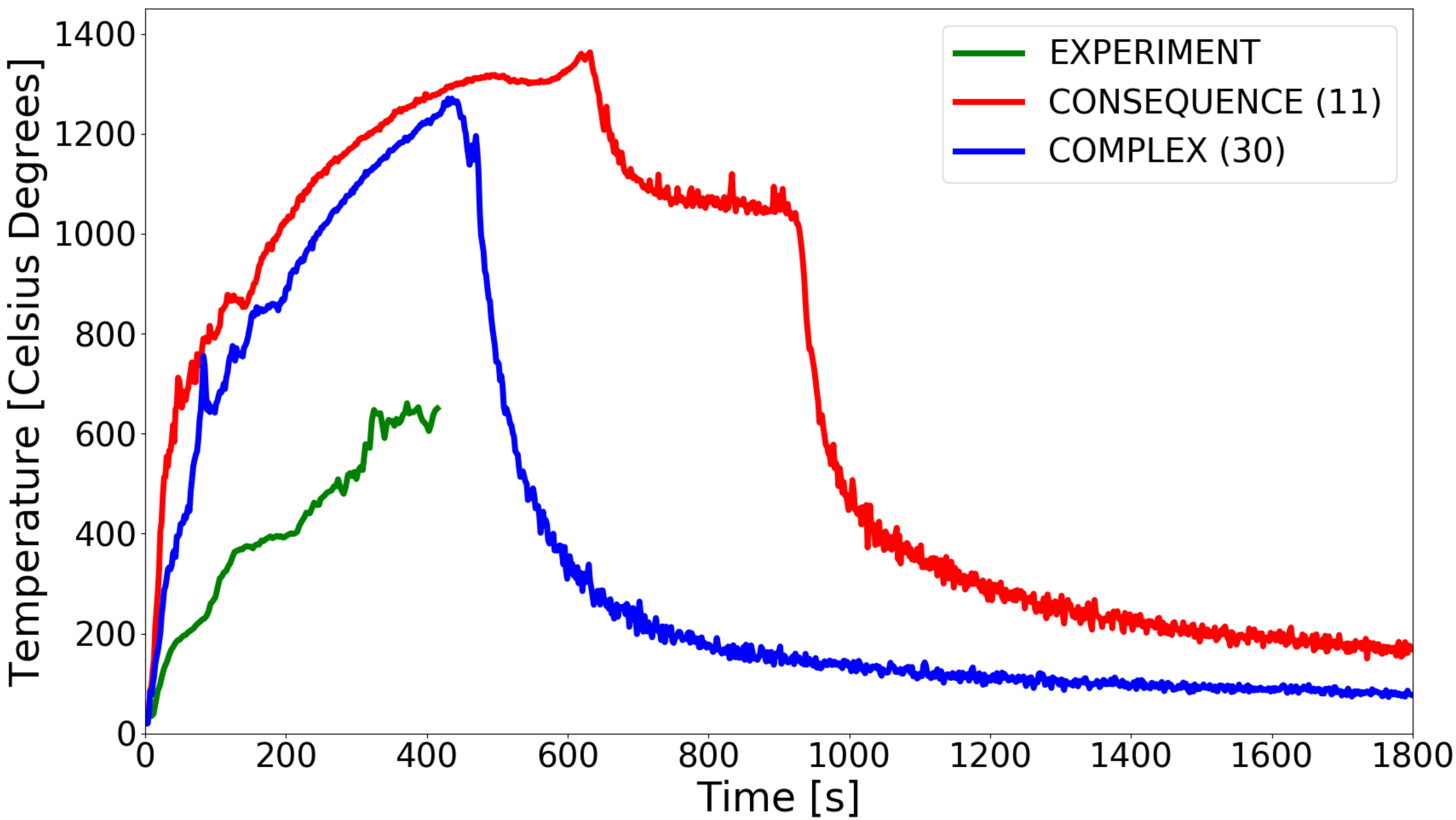
Experimental Data - Thermocouple



Experimental Data - Comparison

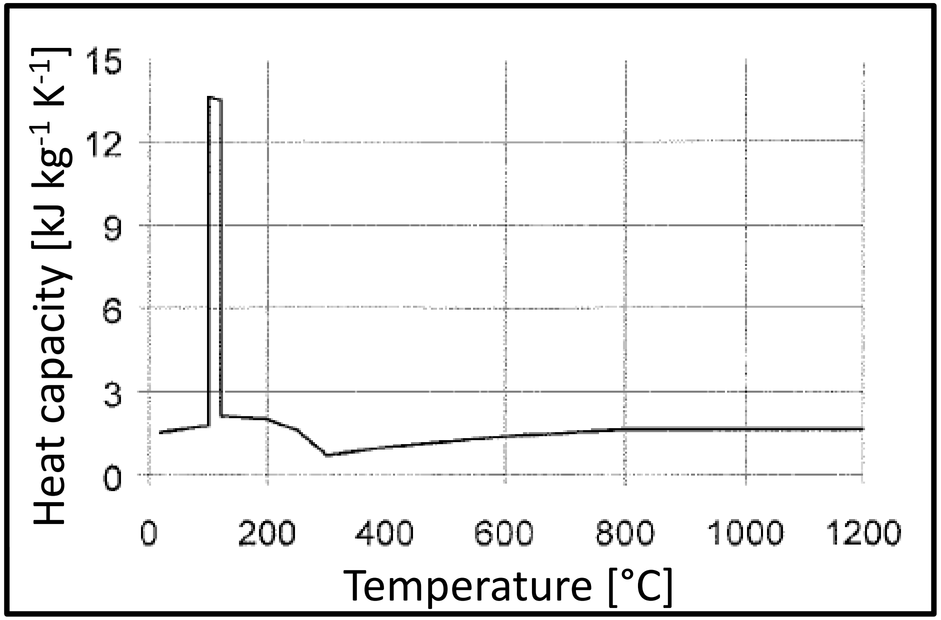


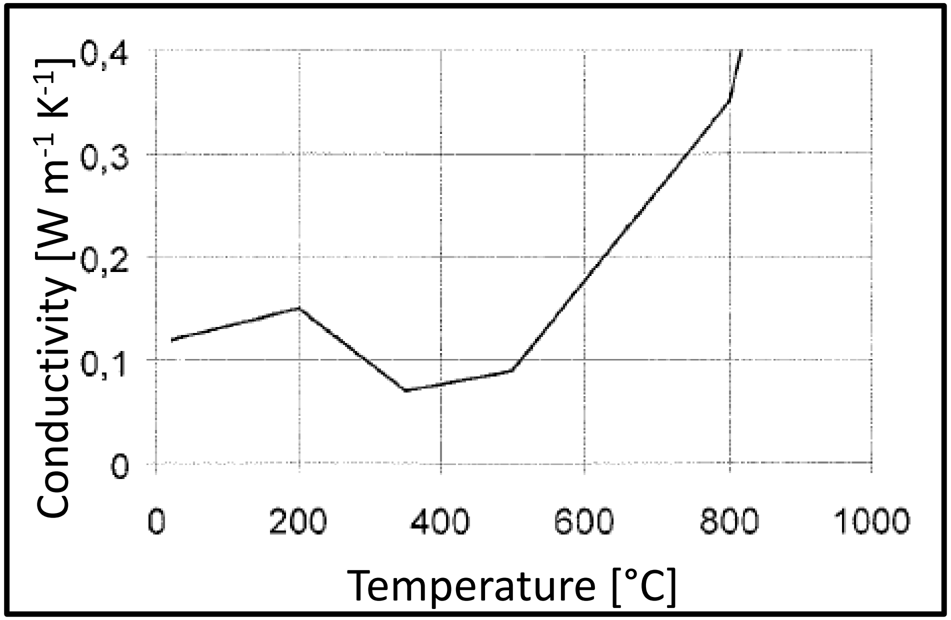
Experimental Data - Comparison



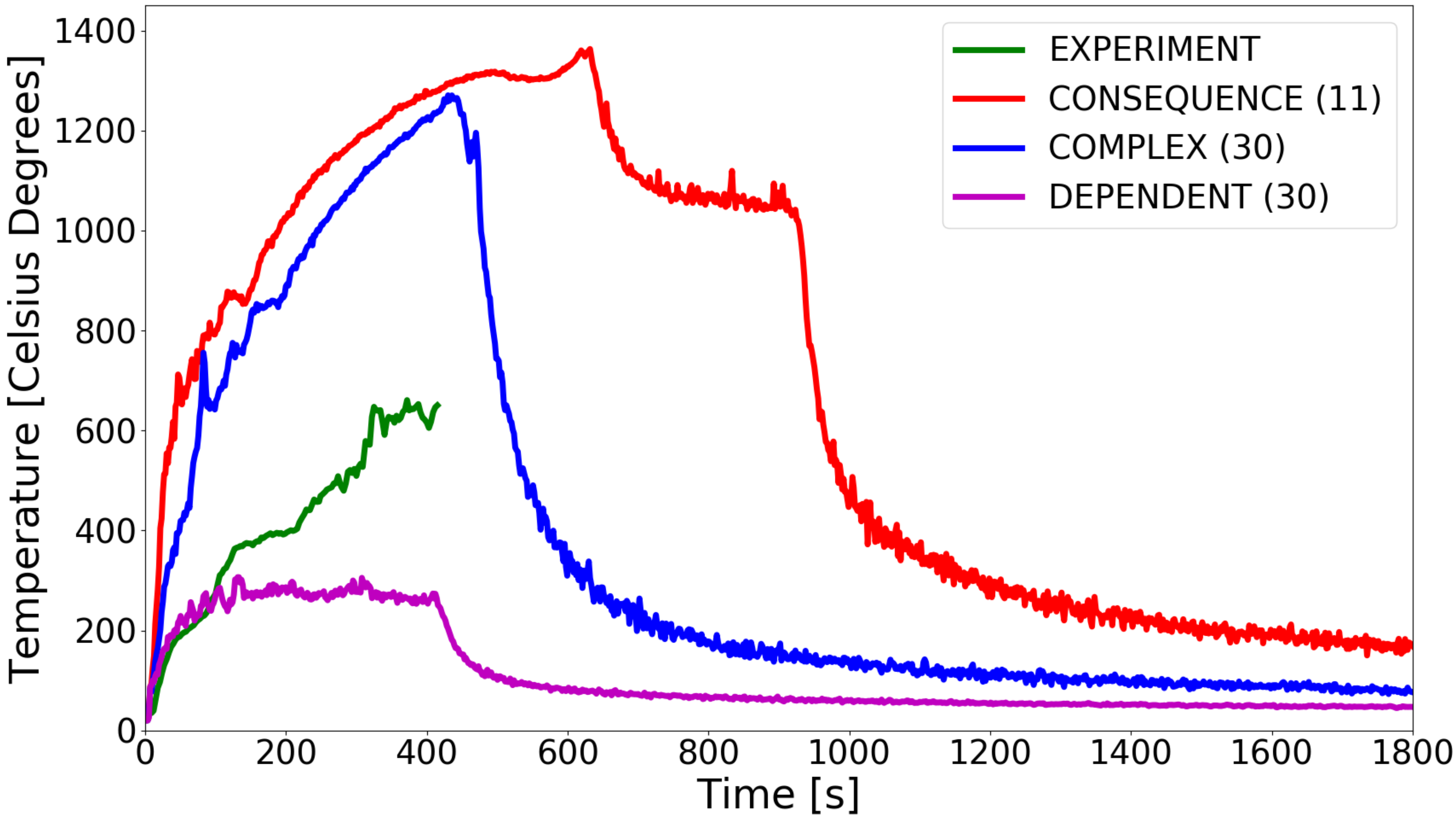
Temperature Dependent Properties

- Eurocode ČSN EN 1995-1-2



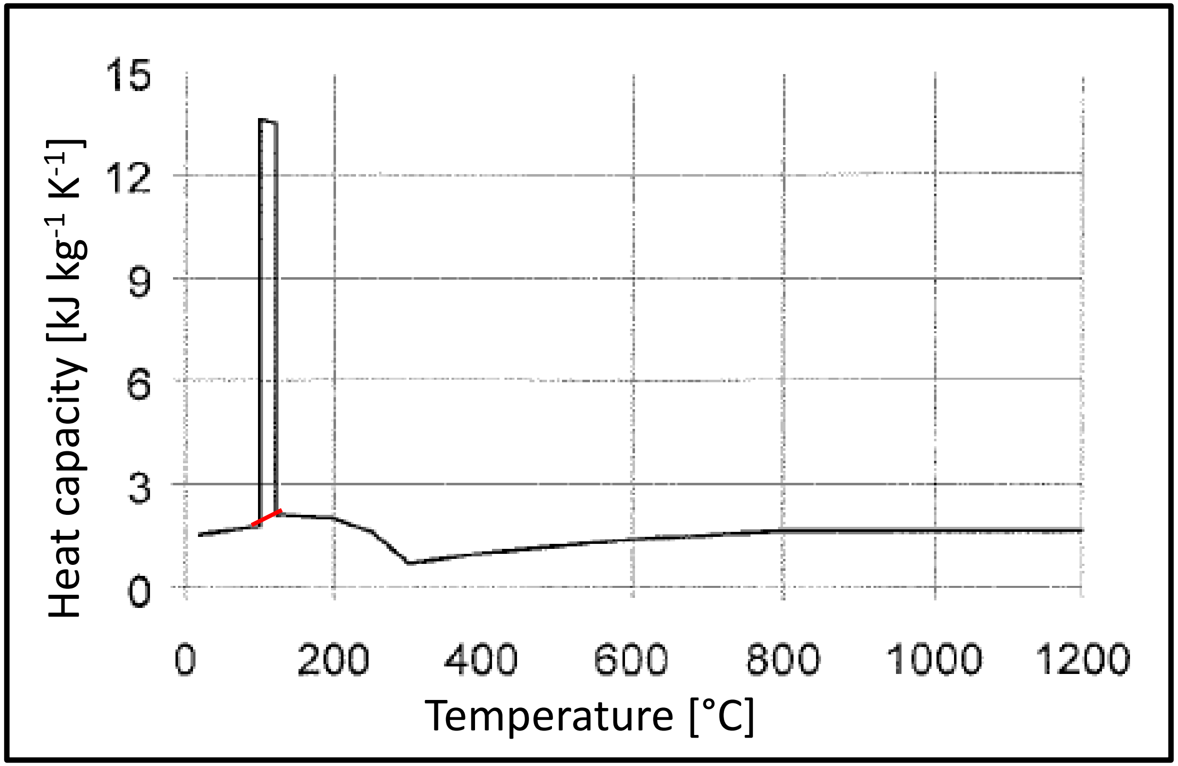


Experimental Data - Comparison

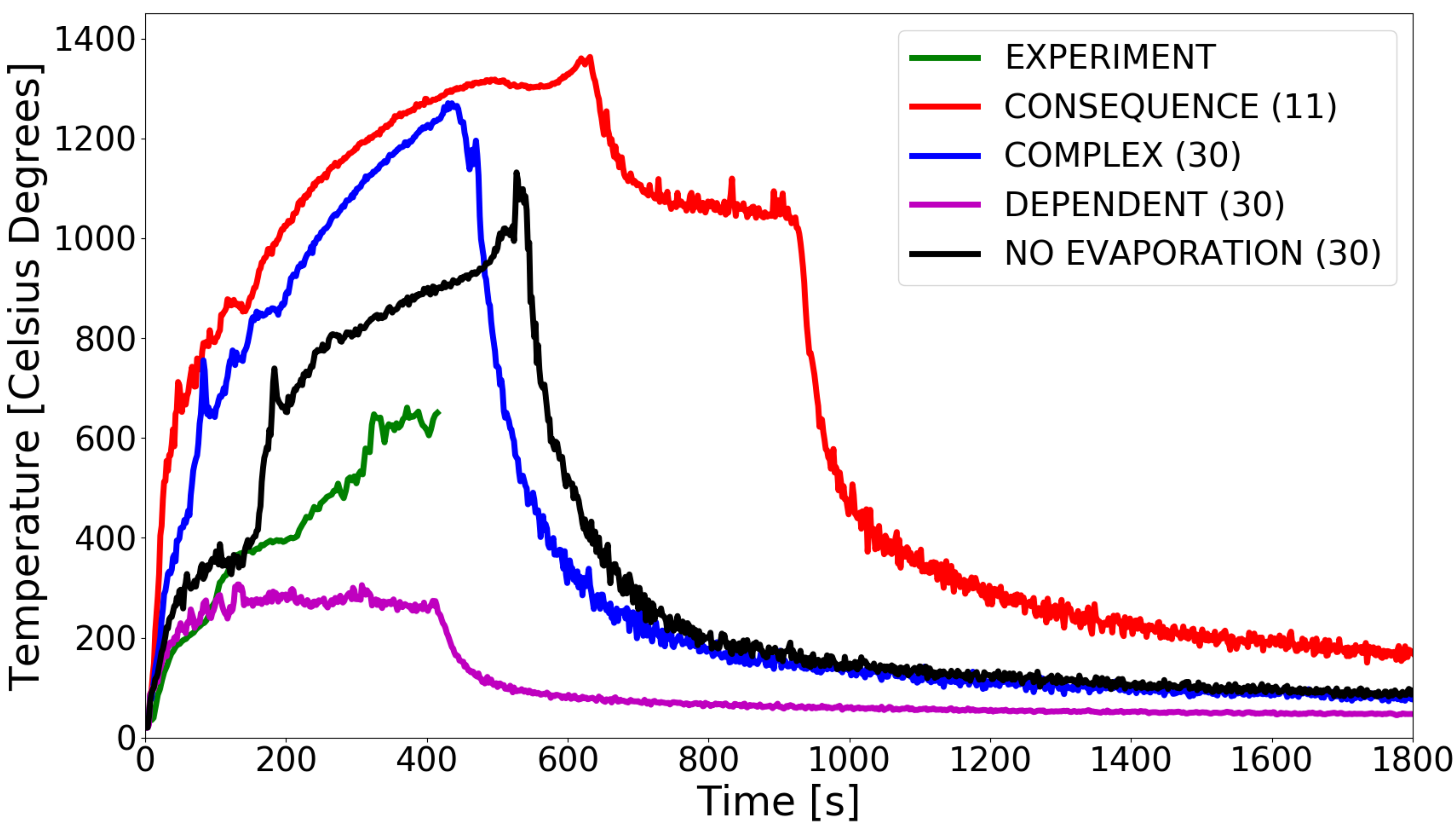


Temperature Dependent Properties

- Eurocode ČSN EN 1995-1-2
- No evaporation



Experimental Data - Comparison



Conclusions and Future Work 2019

- Different pyrolysis models in RCT for OSB board
- HRR modeling insufficient
- Thermal properties most significant

- Thermal properties from cone (PROPTI)
- Coupling with structural solvers
- More detailed char analysis

Conclusions and Future Work 2019

- Different pyrolysis models in RCT for OSB board
- HRR modeling insufficient
- Thermal properties most significant

- Thermal properties from cone (PROPTI) In a minute
- Coupling with structural solvers
- More detailed char analysis

Conclusions and Future Work 2019

- Different pyrolysis models in RCT for OSB board
- HRR modeling insufficient
- Thermal properties most significant

- Thermal properties from cone (PROPTI) In a minute
- Coupling with structural solvers Czech Technical University
- More detailed char analysis

Conclusions and Future Work 2019

- Different pyrolysis models in RCT for OSB board
- HRR modeling insufficient
- Thermal properties most significant

- Thermal properties from cone (PROPTI) In a minute
- Coupling with structural solvers Czech Technical University
- More detailed char analysis ✓

New FDS version 6.7.4

- Update from 6.7.1
- Results differ

FDS 6.7.4 (March 9, 2020)

- Allow particles to follow a `PATH_RAMP(3)` on the `INIT` line; particle `DEVC` output works as usual, so this has the effect of allowing `DEVC` positions to move in time
- Fix bug with FDS+Evac and ZONEs
- Fix bug in mass flux of species at exterior boundaries introduced in v6.7.3 for thin obstructions
- Fix bug that prevented defining an INIT with a species mass fraction of 0 (i.e. override a non-zero `MASS_FRACTION_0` on `SPEC`).
- Fix bug in the initialization of pressure at ambient ducts nodes to correctly use the reference elevation.
- Fix bug in the computation of the initial water vapor mass fraction for `HUMIDITY` .
- Fix bug preventing the use of `TMP_INNER` or `RAMP_T_I` for a particle.
- Generalize histogram generation for regular devices.
- Improve `MEAN_FORCING` functionality by averaging velocity over entire domain, not just entire mesh.
- Allow level set wildland fire fronts to cross mesh boundaries.
- Make baroclinic pressure iteration work with GLMAT pressure solver.

New FDS version 6.7.4

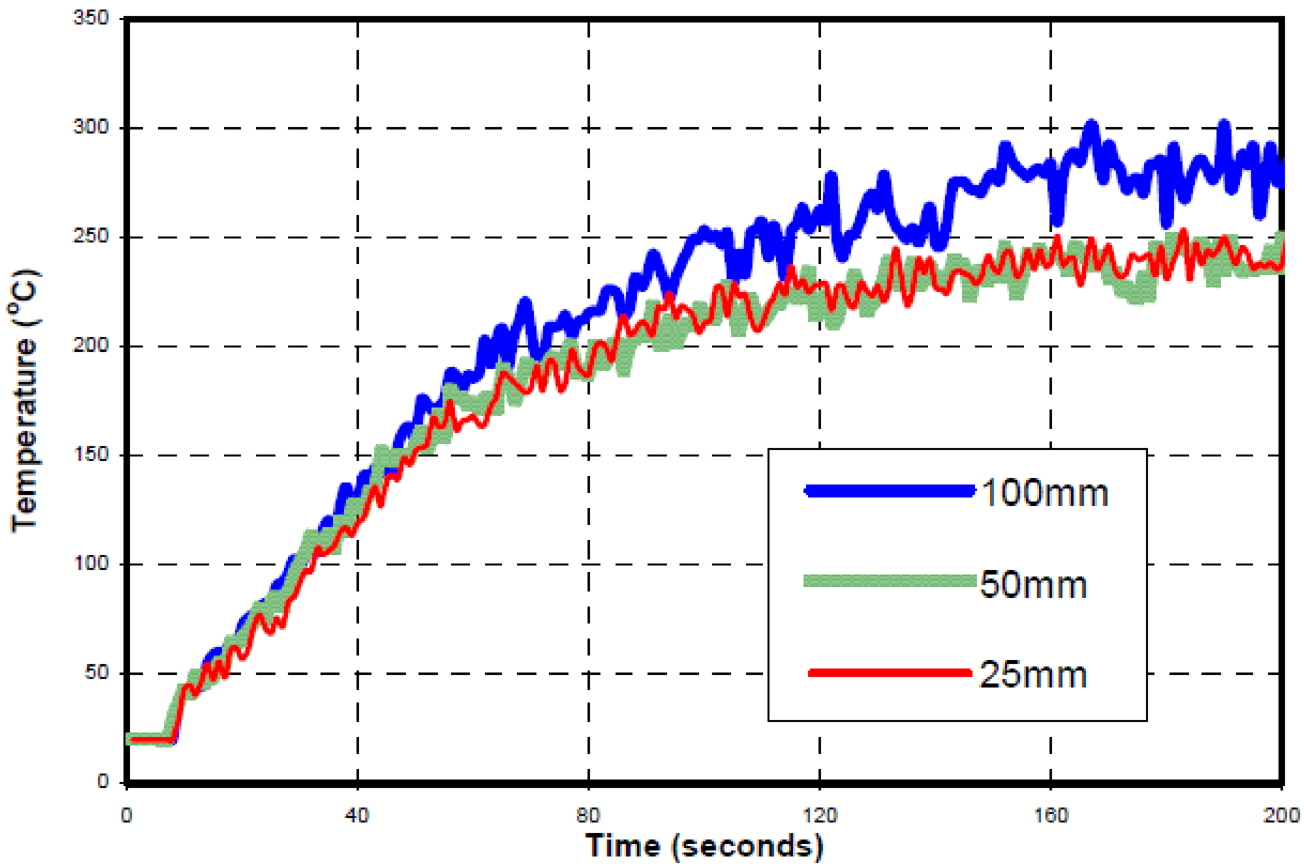
- Solid phase discretization

FDS 6.7.3 (Oct 31, 2019)

- Allow thin obstructions to burn.
- Force explicit setting of mesh transformation `ID` on `MESH` line via `TRNX_ID`, etc. This allows for much greater flexibility in assigning different transformations to different mesh groups for large-scale calculations.
- STRETCH_FACTOR default value set to 2 for all surfaces, even burning surfaces. STRETCH_FACTOR controls the size of solid phase cells used to solve the 1-D heat transfer equation.
- Fixed a bug involving pressure ZONEs. A post to the Forum on June 18th identified a bug where an OBST that formed a boundary between two ZONEs extended over multiple meshes and changed state during the simulation (i.e. had a CTRL_ID or DEVC_ID). As a result of the bug, the ZONEs were not properly initialized.
- Fixed a bug in MIN/MAX CTRL functions.
- Create a `ZONE` using a single `XYZ` point instead of an `XB` volume spanning multiple meshes.
- Increase length of FORMULA (both REAC and SPEC) to 255 characters
- `PATH_RAMP` on `INIT` can specify a path for a particle.
- Added `HEAT_OF_REACTION_RAMP` to `MATL` to specify a temperature dependent heat of reaction.
- Added `RAMP_T_B` to `SURF` to specify a time dependent back wall gas temperature.

Gas phase discretization

- Standard procedure
- Adding cells until they affect results



Moghaddam, A. Z., Moinuddin, K., Thomas, I. R., Bennetts, I. D. and Culton, M. (2004) Fire Behaviour Studies of Combustible Wall Linnings Applying Fire Dynamics Simulator, 15th Australasian Fluid Mechanics Conference.

Solid phase discretization

- Need to solve partial differential equations for heat conduction

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) + \dot{q}_s'''$$

$$-k_s \frac{\partial T_s}{\partial x}(0,t) = \dot{q}_c'' + \dot{q}_r''$$

$$\frac{T_{s,i}^{n+1} - T_{s,i}^{n}}{\delta t}$$

Solid phase discretization

- Need to solve partial differential equations for heat conduction

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) + \dot{q}_s'''$$

$$-k_s \frac{\partial T_s}{\partial x}(0,t) = \dot{q}_c'' + \dot{q}_r''$$

$$\frac{T_{s,i}^{n+1} - T_{s,i}^{n}}{\delta t}$$

- Crank-Nicolson scheme (implicit)

$$(\rho_s c_s)_i \frac{T_{s,i}^{n+1} - T_{s,i}^{n}}{\delta t} = \frac{1}{2 r_{c,i}^J \delta r_i}\left(r_i^J k_{s,i+\frac{1}{2}} \frac{T_{s,i+1}^{n} - T_{s,i}^{n}}{\delta r_{i+\frac{1}{2}}} - r_{i-1}^J k_{s,i-\frac{1}{2}} \frac{T_{s,i}^{n} - T_{s,i-1}^{n}}{\delta r_{i-\frac{1}{2}}} \right)$$
$$+ \frac{1}{2 r_{c,i}^J \delta r_i}\left(r_i^J k_{s,i+\frac{1}{2}} \frac{T_{s,i+1}^{n+1} - T_{s,i}^{n+1}}{\delta r_{i+\frac{1}{2}}} - r_{i-1}^J k_{s,i-\frac{1}{2}} \frac{T_{s,i}^{n+1} - T_{s,i-1}^{n+1}}{\delta r_{i-\frac{1}{2}}} \right) + \dot{q}_{s,i}'''$$

Solid phase discretization

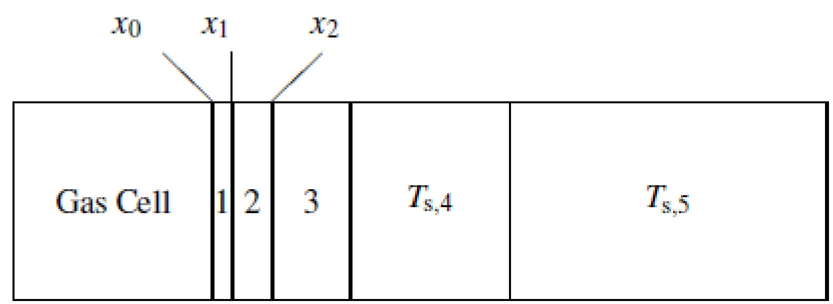
- Need to solve partial differential equations for heat conduction

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) + \dot{q}_s'''$$

$$-k_s \frac{\partial T_s}{\partial x}(0,t) = \dot{q}_c'' + \dot{q}_r''$$

$$\frac{T_{s,i}^{n+1} - T_{s,i}^{n}}{\delta t}$$

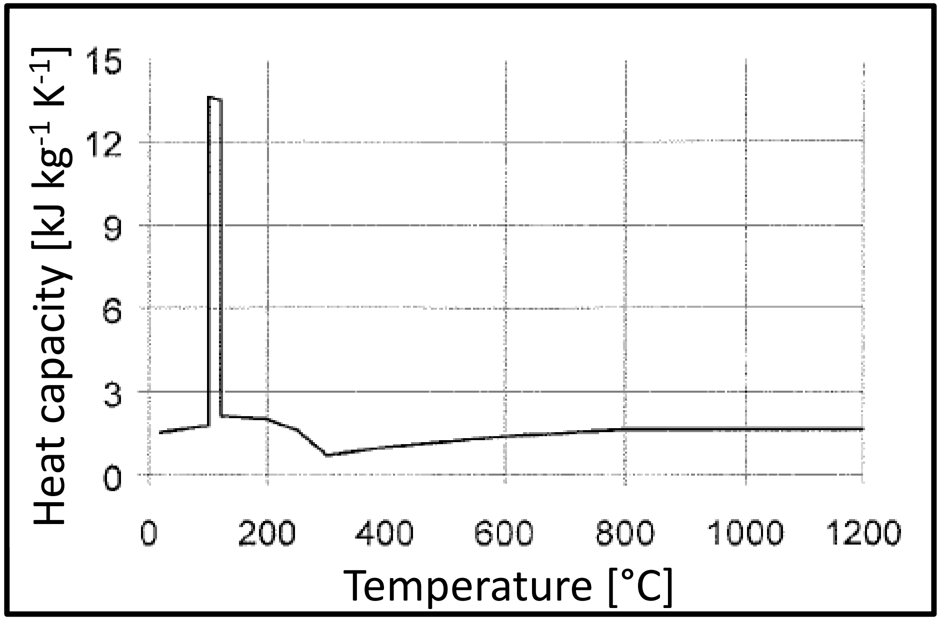
- Default discretization:
  - Wall increment = 2
  - Stretch factor = 2
  - First cell size ≤ $\sqrt{t k_s / \rho c_s}$
  - Cell size factor = 1

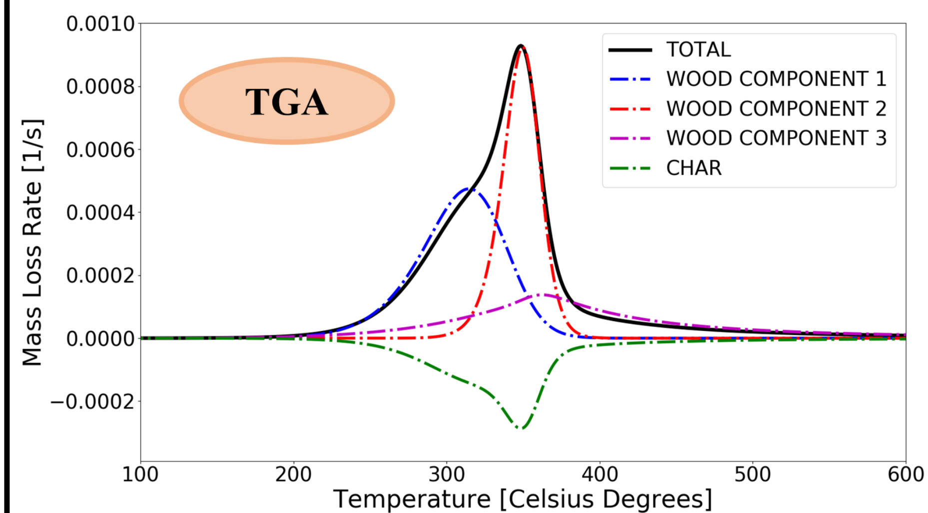


- Why is default not sufficient?

Why is the default not sufficient?

- Reaction rate! (3 pyrolysis reactions)
- Temperature dependent properties





Solid phase discretization

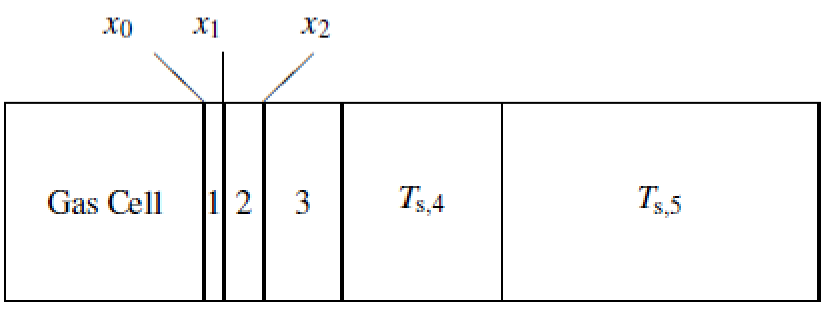
- Need to solve partial differential equations for heat conduction

$$\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) + \dot{q}_s'''$$

$$-k_s \frac{\partial T_s}{\partial x}(0,t) = \dot{q}_c'' + \dot{q}_r''$$

$$\frac{T_{s,i}^{n+1} - T_{s,i}^{n}}{\delta t}$$

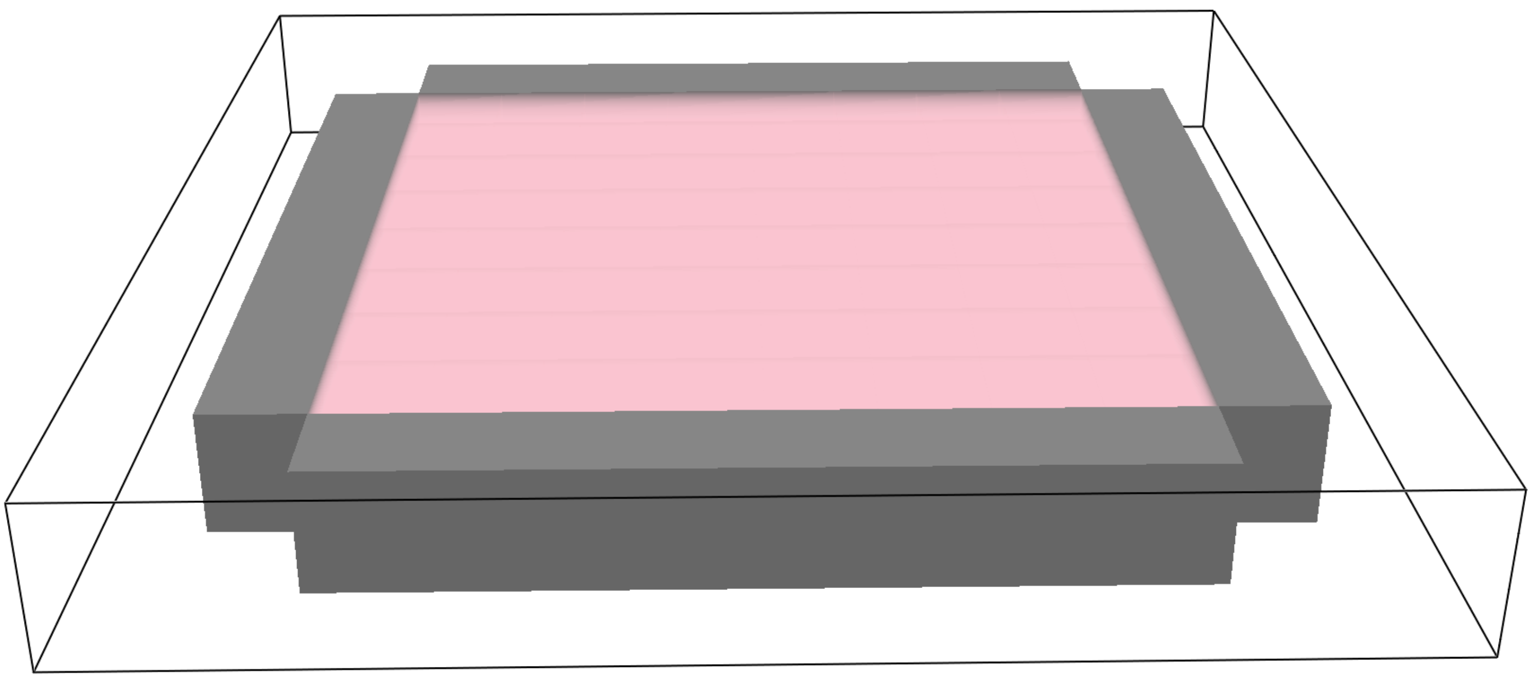
- Default discretization:
    - Wall increment = 2
    - Stretch factor = 2
    - First cell size ≤ $\sqrt{t k_s / \rho c_s}$
    - Cell size factor = 1



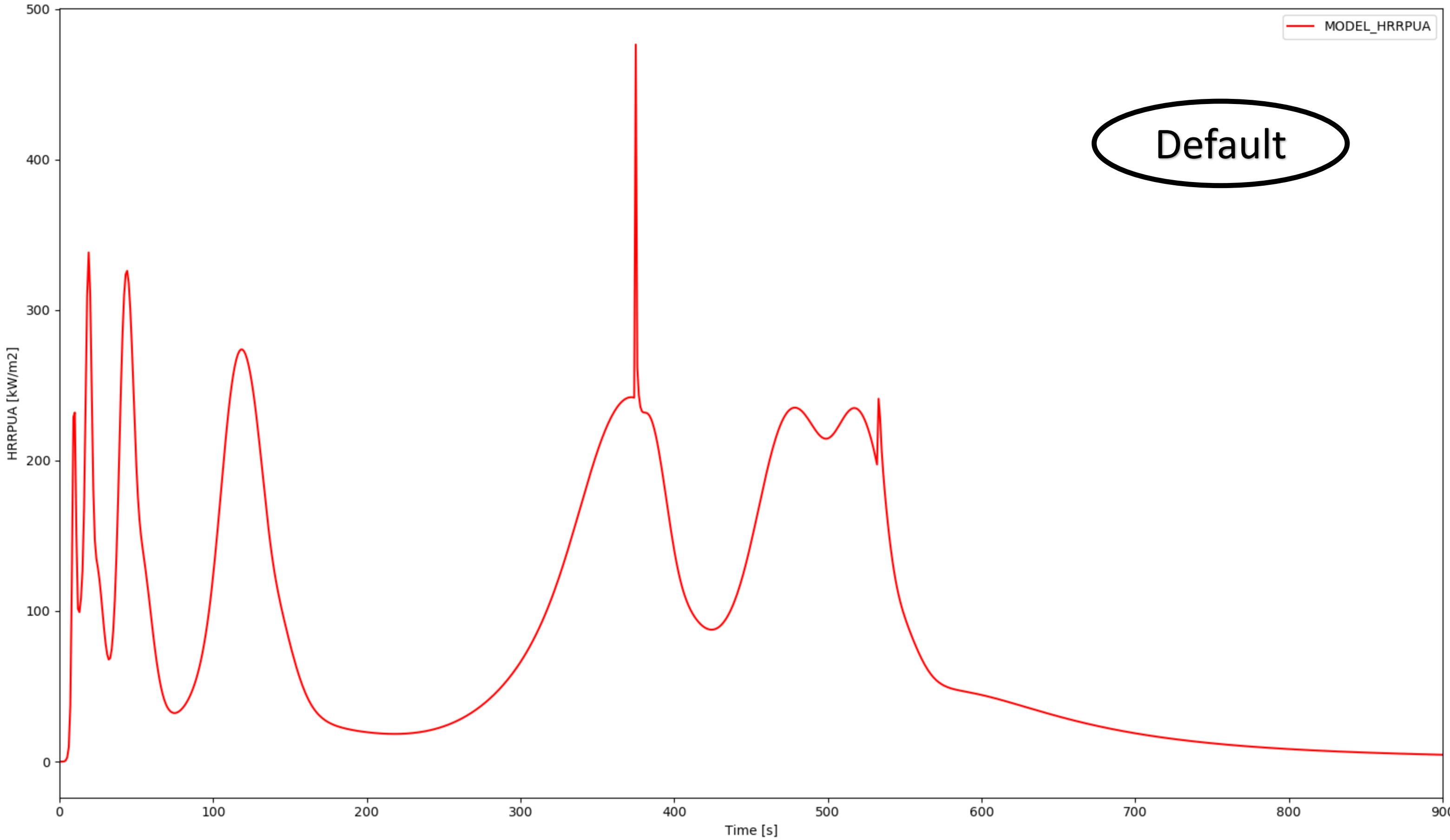
- **Adjusted discretization:**
    - **Wall increment = 1**
    - **Stretch factor = 1**
    - **Cell size factor < 1**
    - **Large increase in computational time**

Solid phase discretization

- Inappropriate to observe solid phase discretization effect from large scale models and from gas phase cells properties
- Focus only on solid phase (solid phase only = true) -> Cone
- Simplest geometry possible

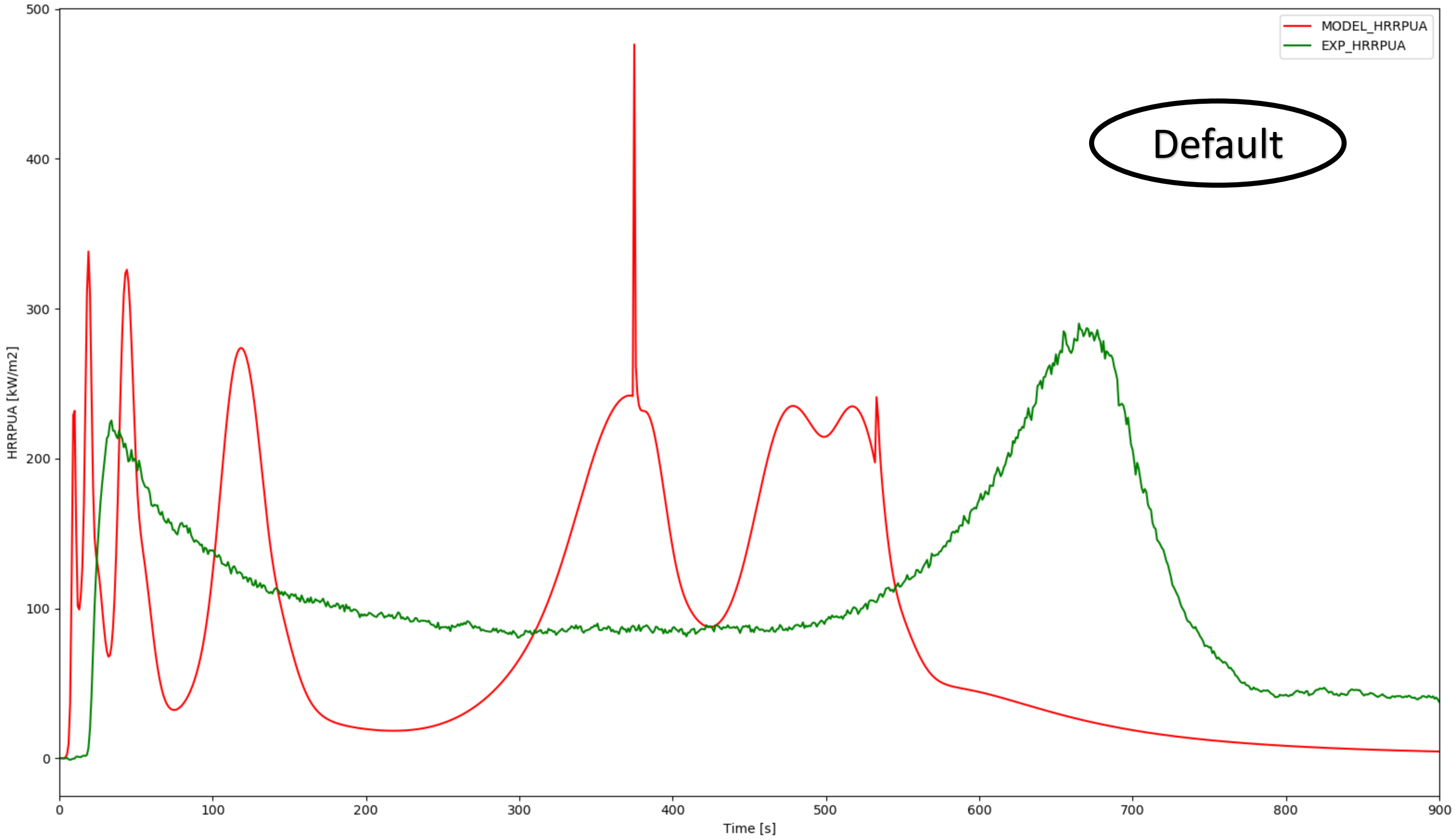


FDS cone calorimetry model



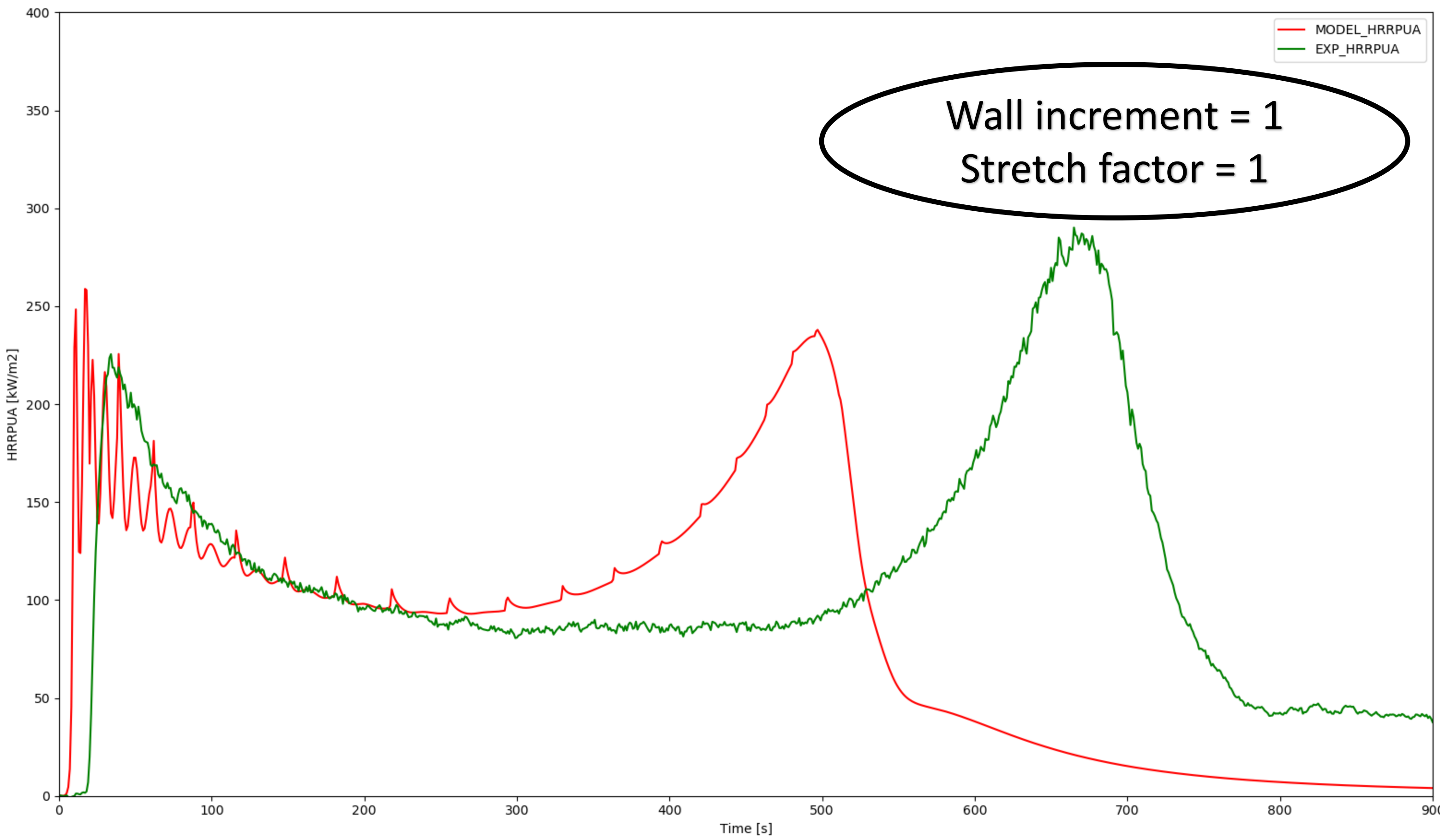
- 50 kW
- 6 sec, 10 cells

FDS cone calorimetry model



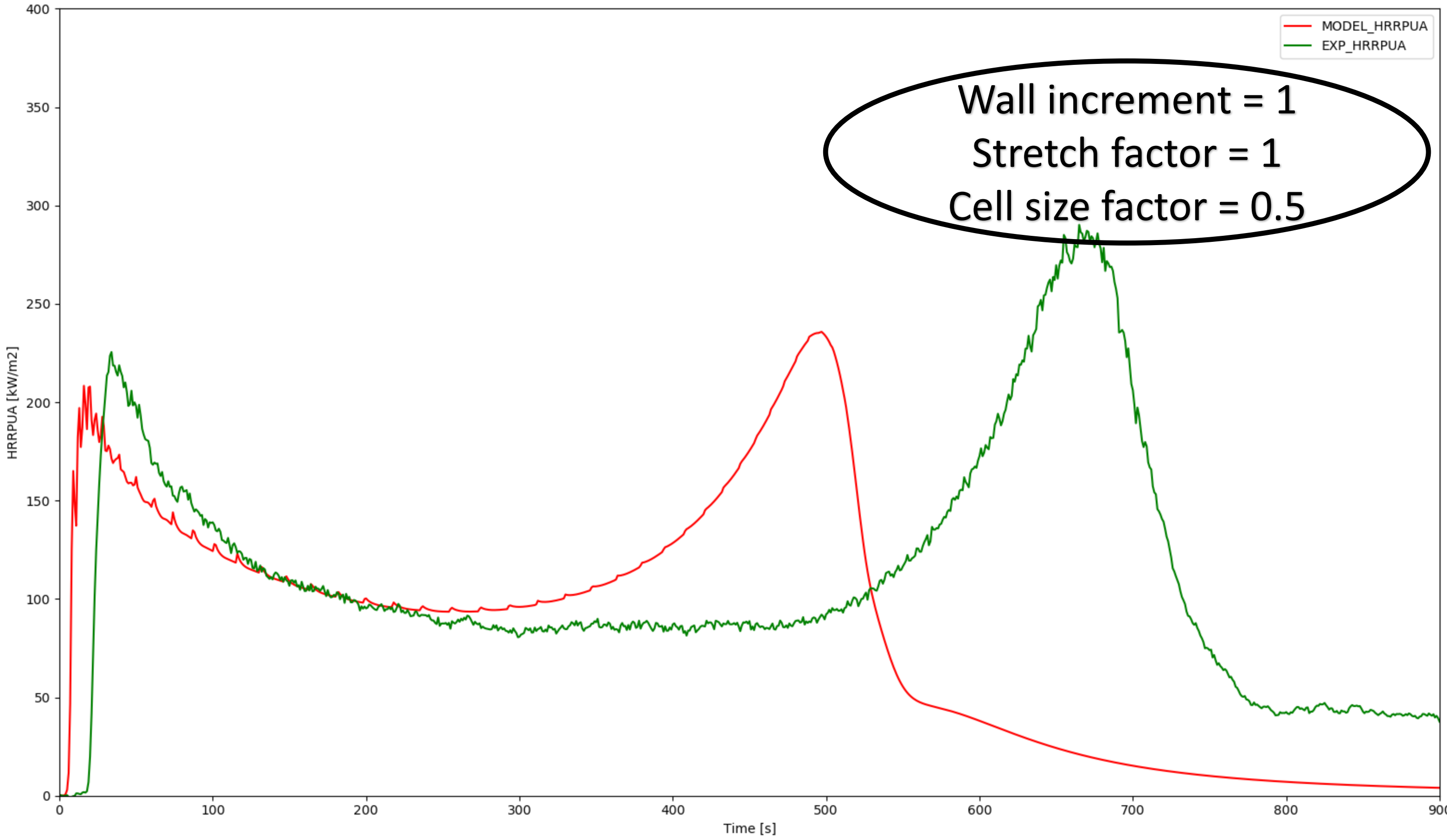
- 50 kW
- 6 sec, 10 cells

FDS cone calorimetry model



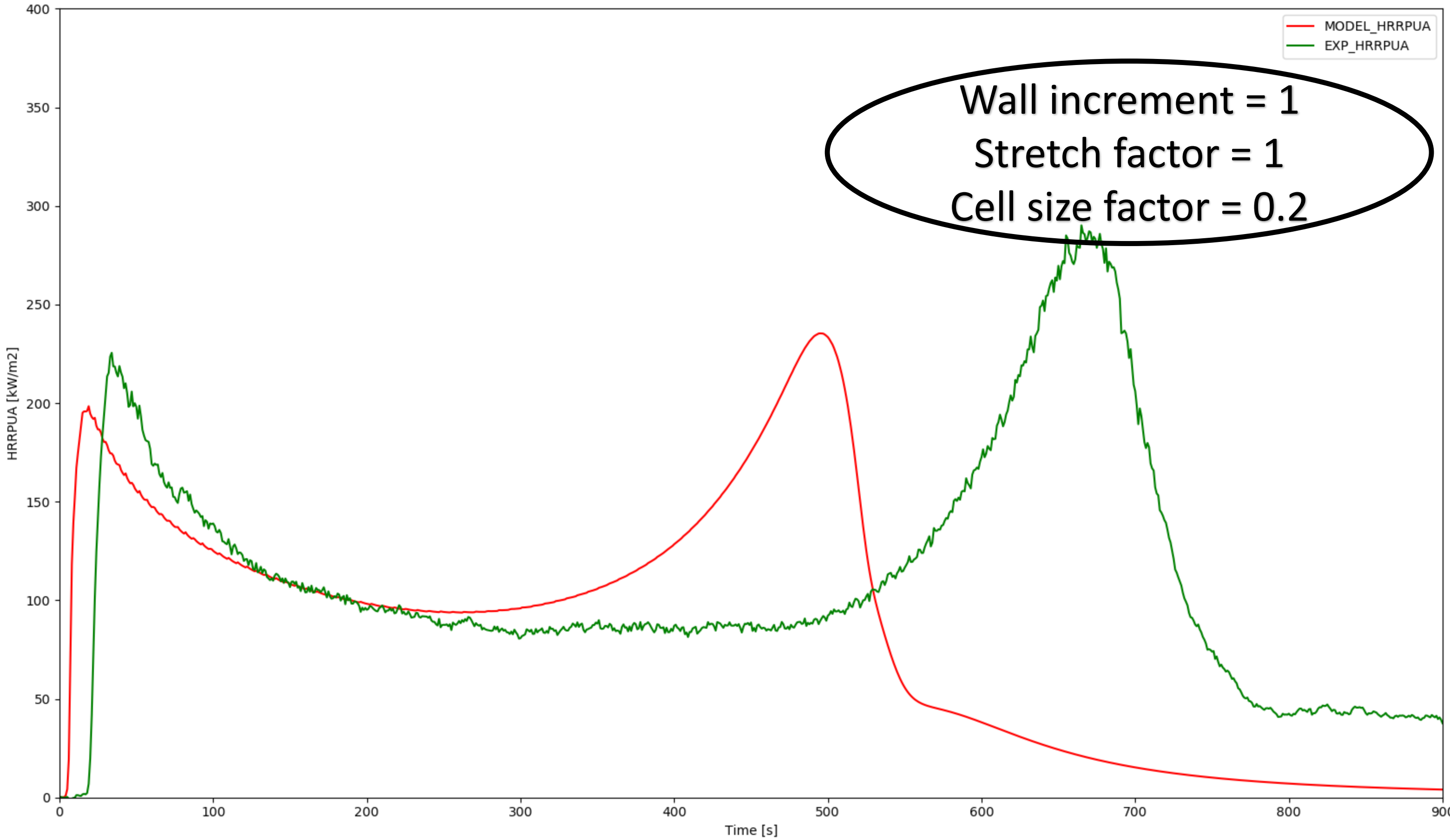
- 50 kW
- 7 sec, 42 cells

FDS cone calorimetry model



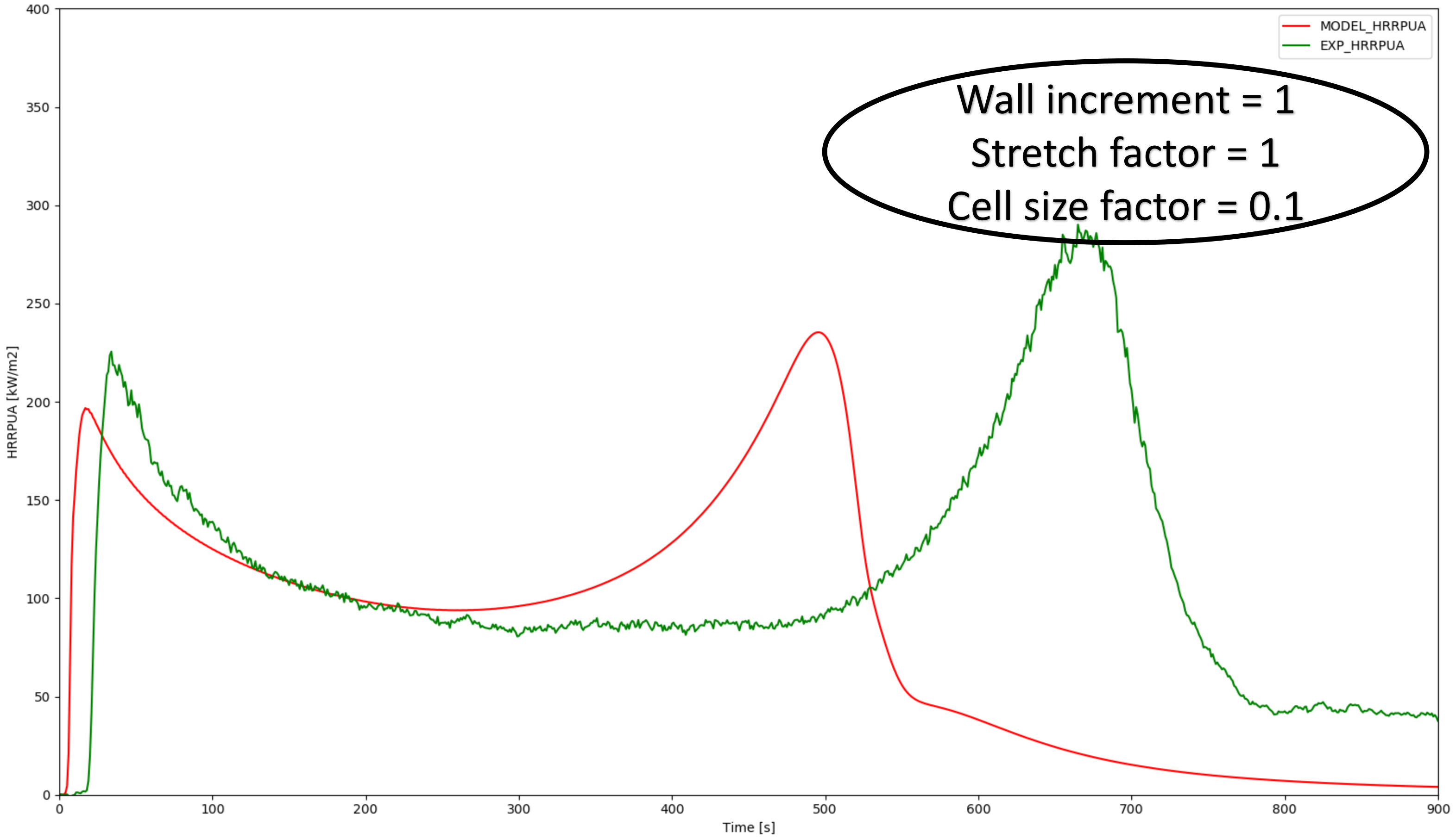
- 50 kW
- 8 sec, 83 cells

FDS cone calorimetry model



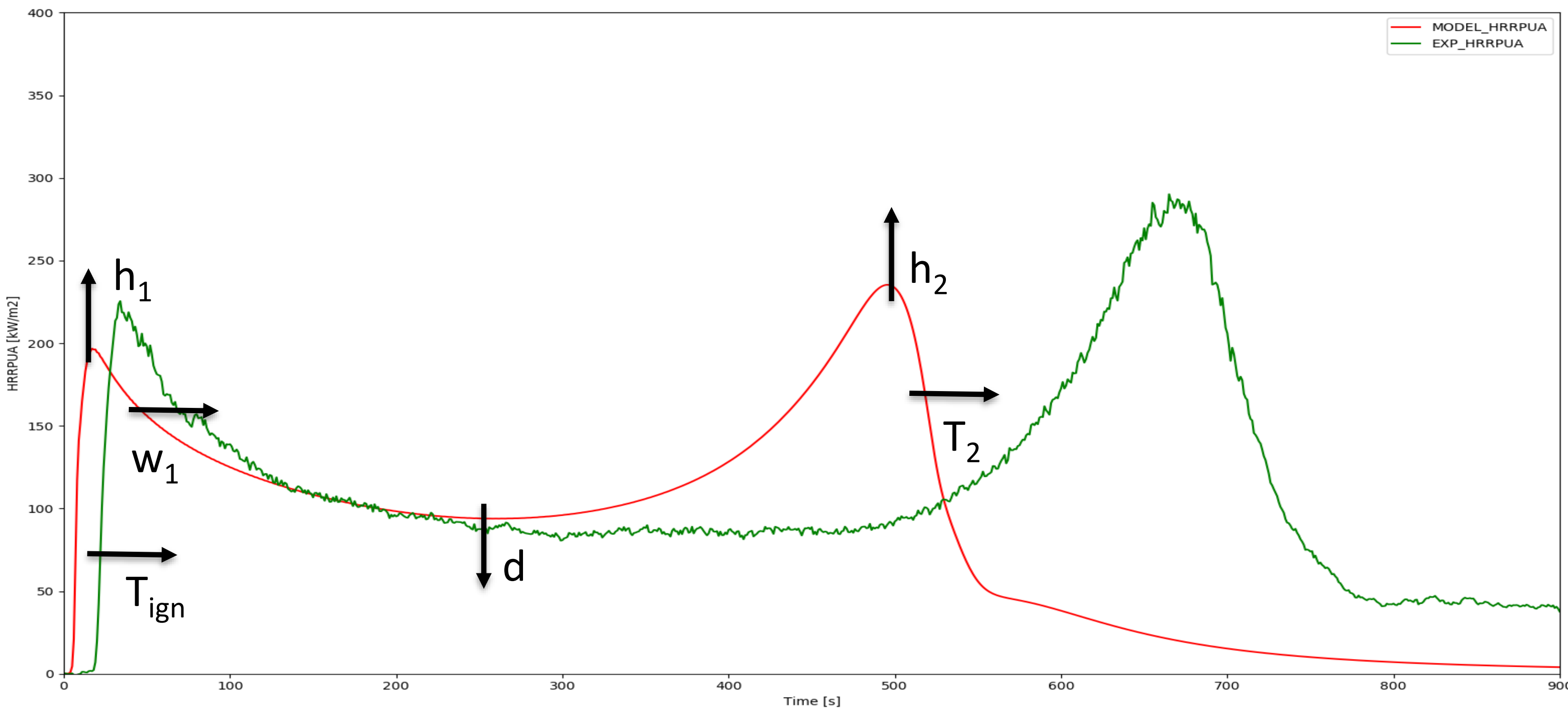
- 50 kW
- 15 sec, 204 cells

FDS cone calorimetry model



- 50 kW
- 42 sec, 407 cells

FDS cone calorimetry model



Effect	k_{solid}	$c_{p,solid}$	k_{char}	$c_{p,char}$	ΔH	ΔH_c
Time of ignition (T_{ign})	+	+	0	0	0	0
1st peak (width) (w_1)	0	0	+	0	(-)	0
1st peak (height) (h_1)	0	0	0	0	(-)	+
Depth of valley (d)	0	+	-	0	+	+
2nd peak (time) (T_2)	-	+	-	0	0	+
2nd peak (height) (h_2)	+	+	+	-	-	+

FDS - PROPTI cone calorimetry model

- Optimization, analogy to kinetics from TGA data
- Selection of searched parameters
  - **c_s of char** <0.2; 2.0> (literature 0.8)
  - **k_s of char** <0.02; 0.3> (literature 0.1)
  - **c_s of all 3 wood components** <0.3; 3> (literature 1.221)
  - **k_s of all 3 wood components** <0.02; 0.3> (literature 0.098)

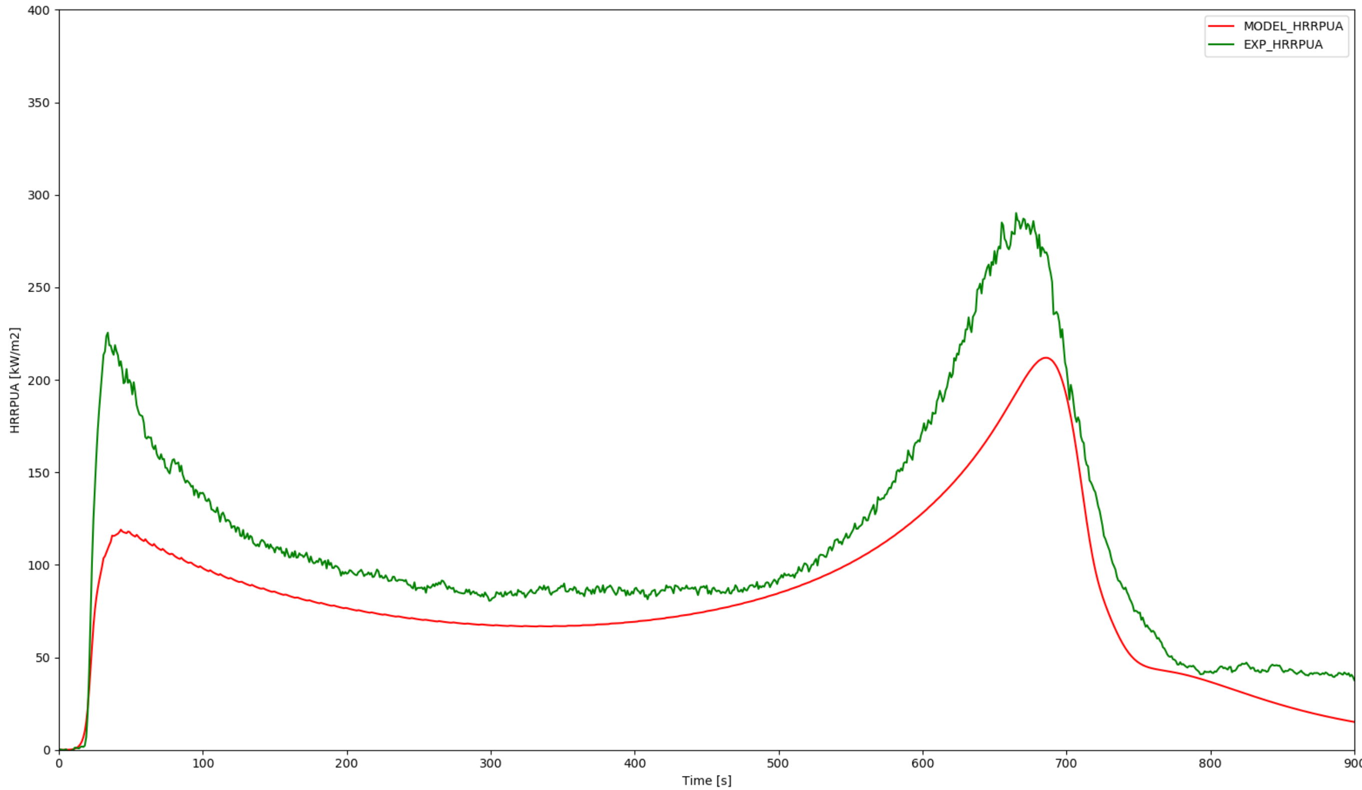
```
&MATL ID='LIGNIN',
      SPECIFIC_HEAT=#Cp_01#,
      CONDUCTIVITY=#K_01#,
      DENSITY=587.1,
      N_REACTIONS=1.,
      A(1)=38018940.,
      E(1)=112460.,
      N_S(1)=1.21,
      MATL_ID(1,1)='CHAR',
      NU_MATL=0.2306,
      SPEC_ID(1,1)='REAC_FUEL',
      NU_SPEC(1,1)=0.7694,
      HEAT_OF_REACTION=77.7,
      HEAT_OF_COMBUSTION=11710. /
```

```
&MATL ID='CHAR',
      SPECIFIC_HEAT=#Cp_CH#,
      CONDUCTIVITY=#K_CH#,
      DENSITY=299.0/
```

```
# use default values for optimiser
optimiser = pr.OptimiserProperties(algorithm='sceua',
                                   repetitions=10000,
                                   ngs=4,
                                   backup_every=100)
```

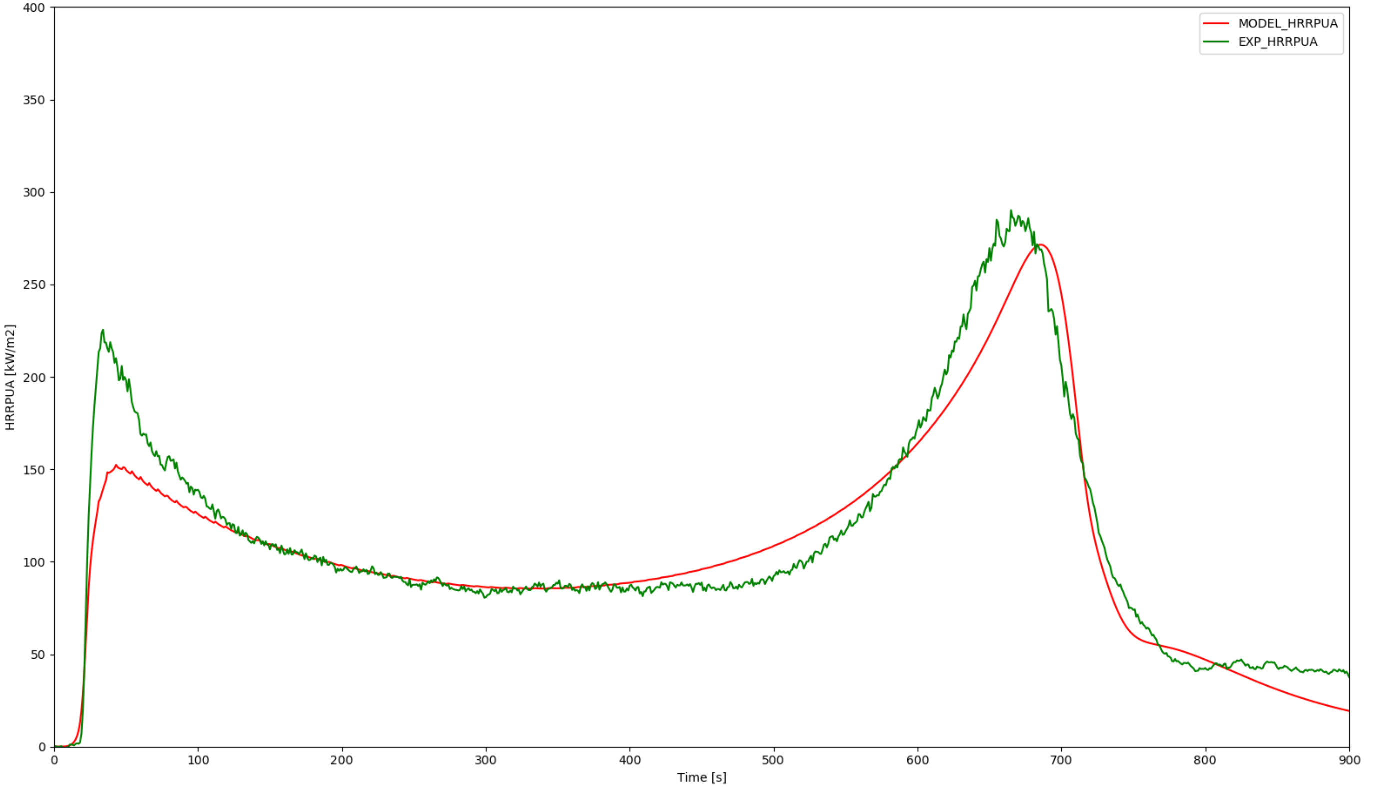
FDS - PROPTI cone calorimetry model

- Optimized parameters (from 50 kW)
  - c_s of char **0.204** (literature 0.8)
  - k_s of char **0.104** (literature 0.1)
  - c_s of all 3 wood components **2.509** (literature 1.221)
  - k_s of all 3 wood components **0.177** (literature 0.098)

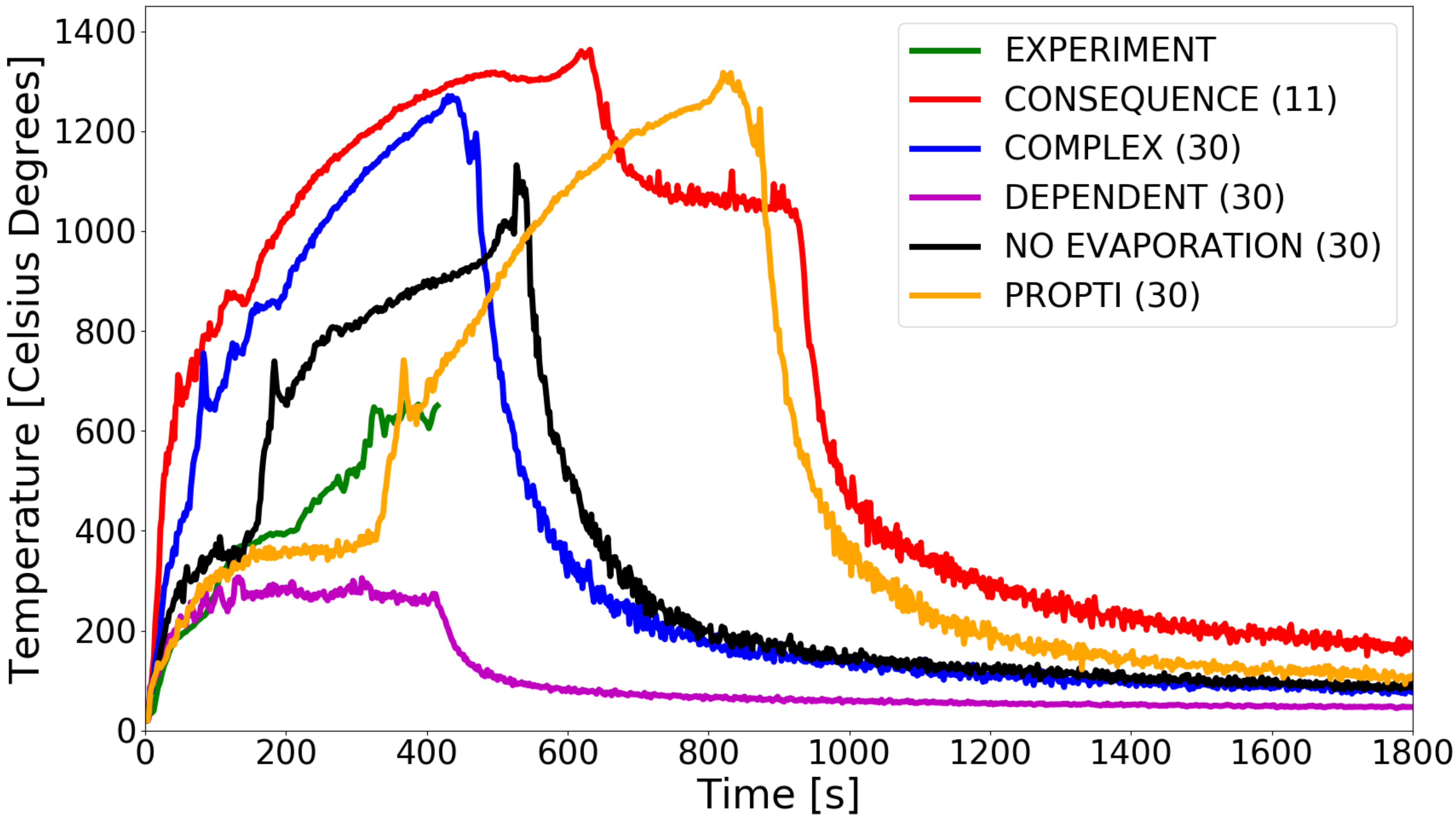


FDS - PROPTI cone calorimetry model

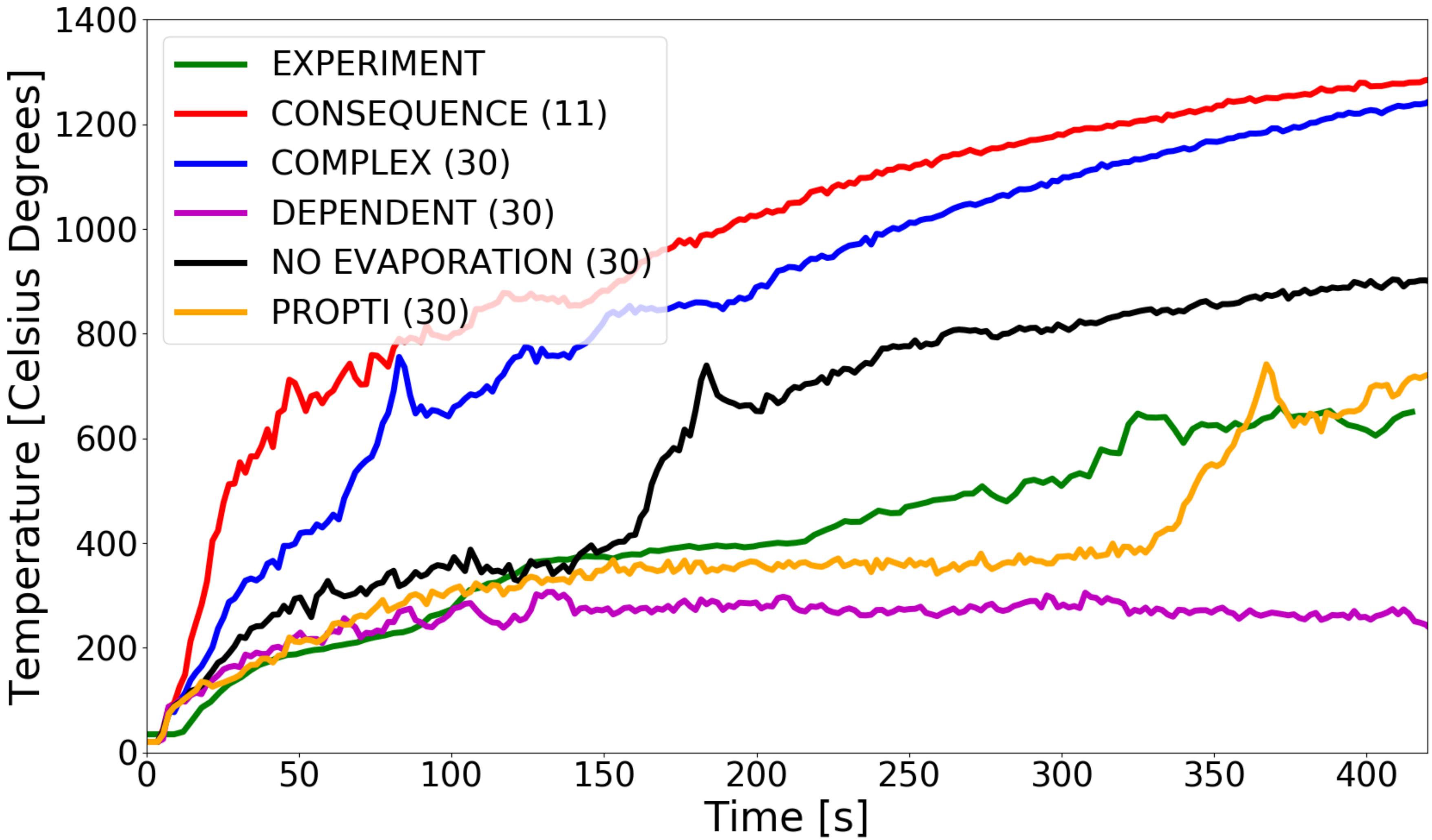
- c_s of char **0.222** (literature 0.8)
- k_s of char **0.083** (literature 0.1)
- c_s of all 3 wood components **2.356** (literature 1.221)
- k_s of all 3 wood components **0.179** (literature 0.098)
- ΔH_C of all 3 wood components **15756** (experiment 11710)



Experimental Data - Comparison



Experimental Data - Comparison



Conclusions and Future Work

- Solid phase discretization
- Promissing RCT model outputs using PROPTI

- Thermal properties from cone at different heat flows (PROPTI)
- Different materials (spruce, chipboard)
- More detailed cone model using HT3D and char properties

Thank you for your attention

This work was supported from the grant of Specific university research – grant No A2_FCHI_2020_012 and by the Ministry of Interior, Safety research Programme of the Czech Republic 2015 – 2022 (BV III/1-VS) under number VI3VS/741 - Fire development modelling of engineered wood.