A CFD model for the smoldering combustion of the cellulosic substrate during the IP test

MSc. Apurva Patel
Dr. Torsten Kolb
Dr. Pablo Guindos

Fraunhofer WKI
38108 Braunschweig
Germany

Custom Order of the Presentation

I. Main Output

II. Motivation and Objective

III. Experimental Characterization of the Substrate

IV. Numerical Model of the Substrate

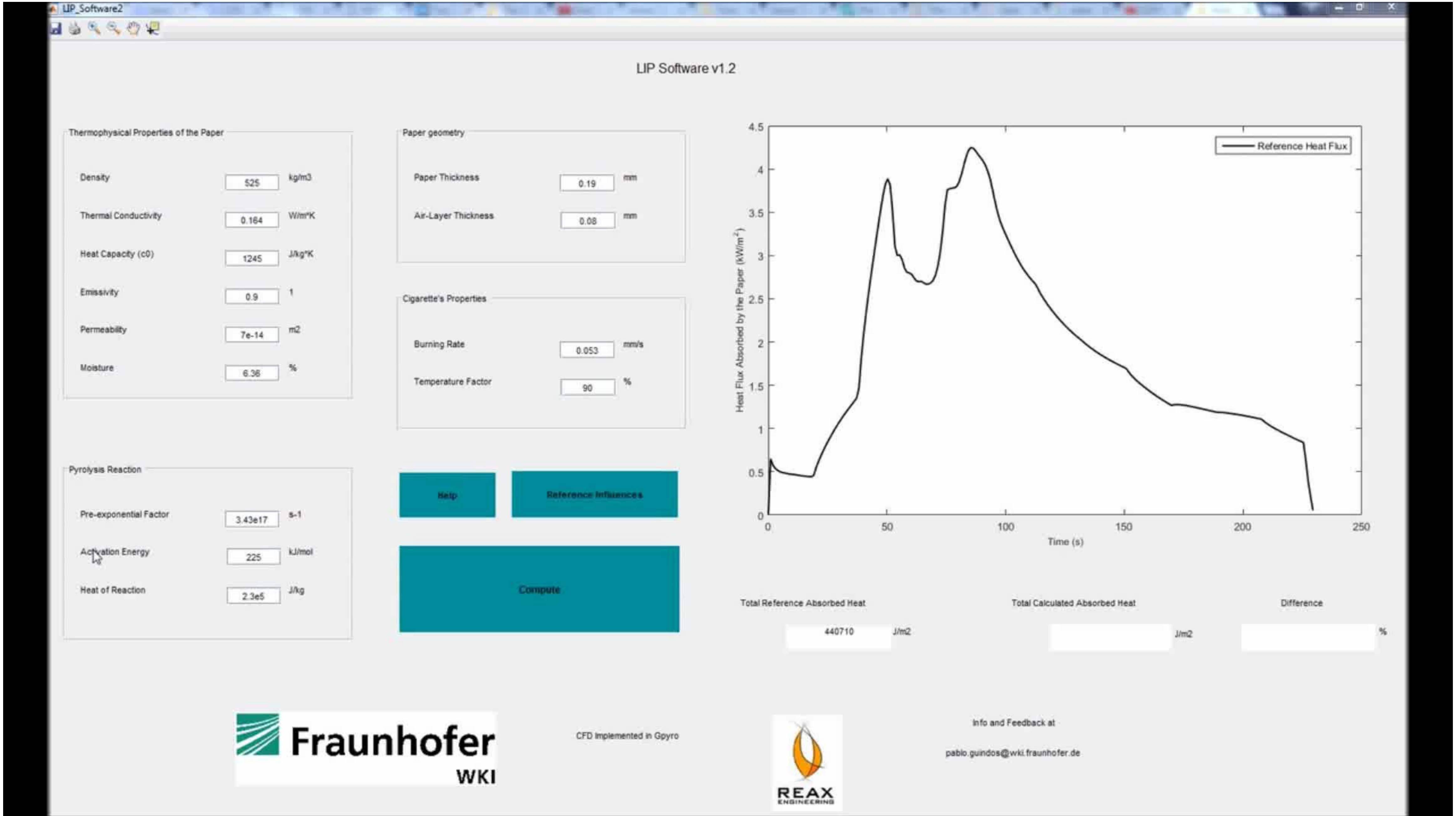
V. Analysis of the Substrate

VI. SIMULIP Software v1.2

VII. Conclusion

Fraunhofer
WKI

Main Output: SIMULIP Software v1.2



Motivation

- Poor repeatability of the tests
  - Difficult to understand
  - Difficulties to improve design of cigarettes
- Relatively expensive in time and money

Objective

- How does the substrate influence the IP tests?
- What are the thermodynamic properties of the substrate?
- What are the most influencing properties of the substrate and how are they influencing?
- Is the poor repeatability of the test exclusively due to the variability of the cigarettes?
- In case an alternative substrate is to be used, what should its characteristics be?

Scientific Approach

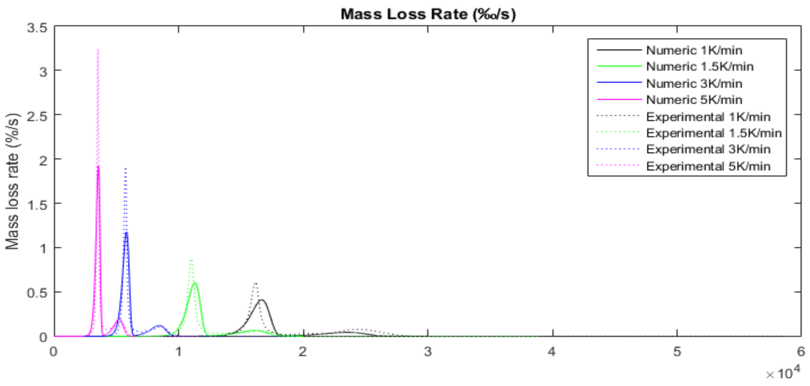
1. Characterize the thermodynamic properties of the Whatman Paper ® no. 2
2. Create a mathematical model based on the physics of the problem.
3. Validate the model against experiments.
4. Analyze the potential influence of the substrate with the model.
5. Analyze what the difference if would be if using an alternative substrate with the model.

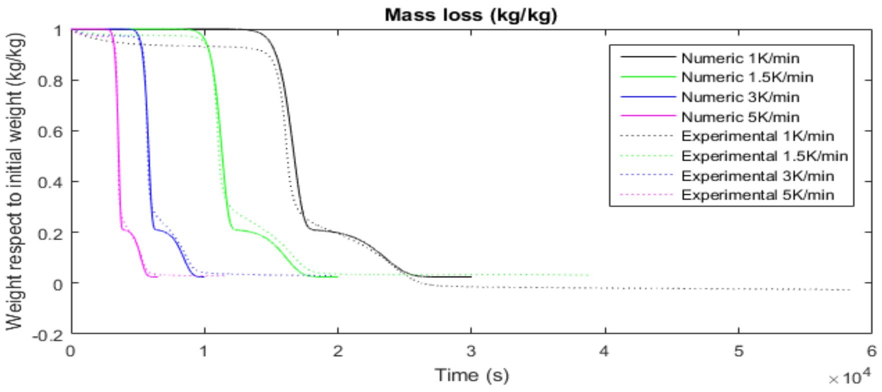
Characterization of the substrate: Summary

Property	Method	No. of tests	Mean (±SD)
Paper thickness (μm)	ISO 534 [7]	20	191 ± 7
Air layer thickness (μm)	Laser triangulation	1	80
Paper density (g/m^3)	ISO 534 [7]	20	0.525 ± 0.021
Moisture content (%)	ISO 287 [6]	20	6.360 ± 0.078
Char mass fraction (1)	TGA+SCE	9	0.21
Ash mass fraction (1)	TGA+SCE	9	0.02
Specific volume (m^3/g)	ISO 534 [7]	20	1.909 ± 0.078
Grammage (g/m^2)	ISO 536 [8]	20	99.915 ± 0.92
Permeance (μm/Pa·s)	ISO 5636-3 [9]	10	25.7 ± 1.14
Permeability (m^2)	Calculated from permeance	10	$7.29 \cdot 10^{-14}$
Thermal conductivity (W/mK)	THB	8	0.164 ± 0.011
Heat capacity (J/kgK)	DSC	4	Eq. 1
Pre-exponential factor of pyrolysis (s^{-1})	TGA+SCE	9	$3.4 \cdot 10^{17}$
Activation energy of pyrolysis (kJ/mol)	TGA+SCE	9	225
Heat of the pyrolysis (kJ/kg)	DSC	4	230
Pre-exponential factor of char oxidation (s^{-1})	TGA+SCE	9	$1 \cdot 10^{8}$
Activation energy of char oxidation (kJ/mol)	TGA+SCE	9	140
Heat of char oxidation (kJ/kg)	DSC/Literature [11]	-	$-25 \cdot 10^{3}$
Gross heat of combustion (kJ/kg)	ISO 1716 [5]	1 (500g)	16808
Net heat of combustion (kJ/kg)	ISO 1716 [5]	1 (500g)	15432
Roughness at the upper (A) and lower (B) sides (ml/min)	ISO 8791-2 [10]	10	A=1685 ± 88.4 B=1165 ± 41.2
Elemental analysis (%)	IRMS	3	C = 42.906 ± 0.043 H = 6.465 ± 0.040 N = 2.829 ± 0.462 S = 0.303 ± 0.071

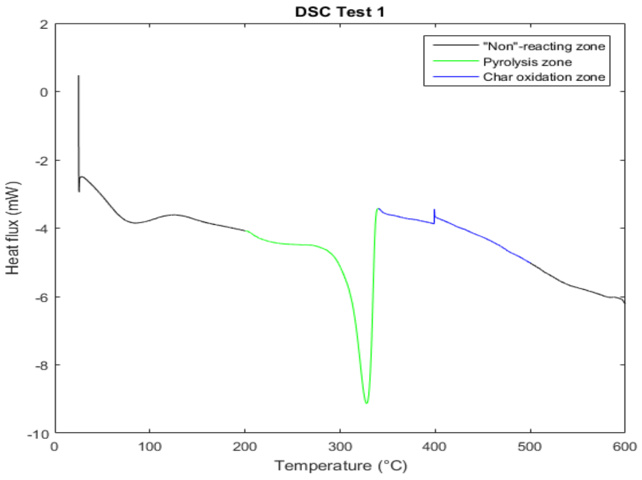
Characterization of the substrate: Chemical Kinetics Experiments

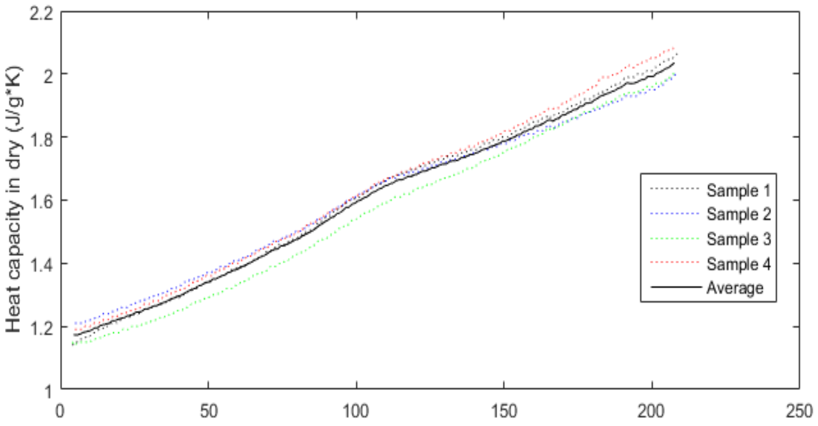
1. Thermogravimetric Analysis (TGA) + Shuffled Complex Evolution = Pre-exp. Factor + Activation Energy





2. Differential Scanning Calorimetry (DSC) + Fitting and Integration = Heat Capacity + Heat of Reactions





$$c_{p,c} = c_{p,c,25^oC} \cdot \left(\frac{T}{298} \right)^{1.037}$$

R^2=0.9965

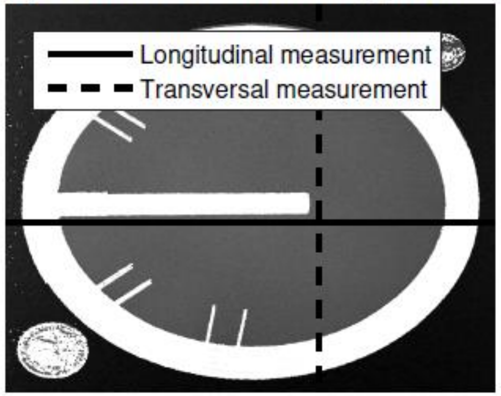
Fraunhofer WKI

Characterization of the substrate: Air Gap Thickness

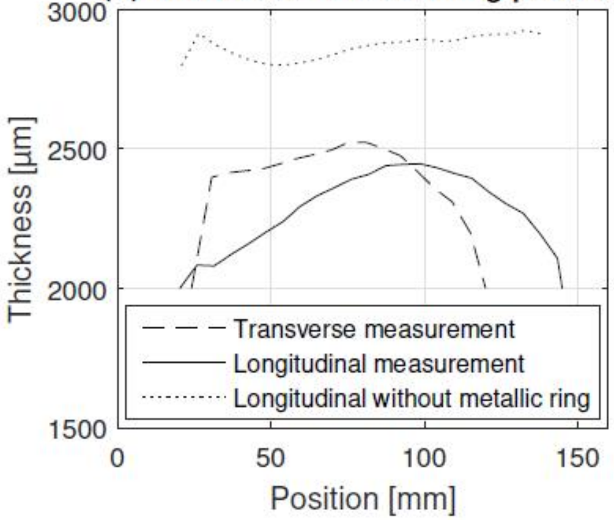
(a) Components of the IP test

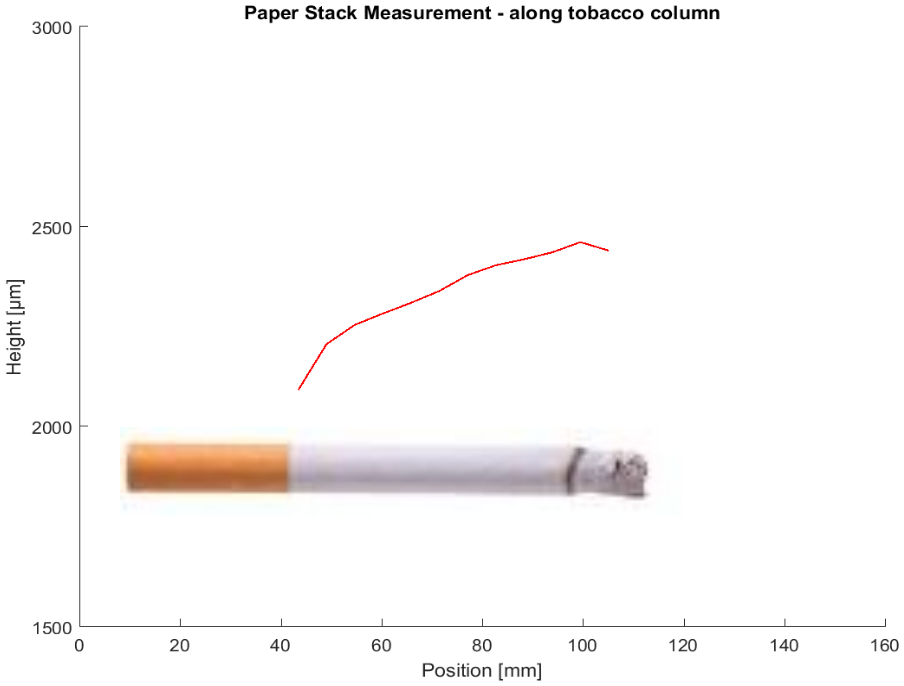
(b) IP test set up

(c) Position of measuring profiles



(d) Thickness of measuring profiles

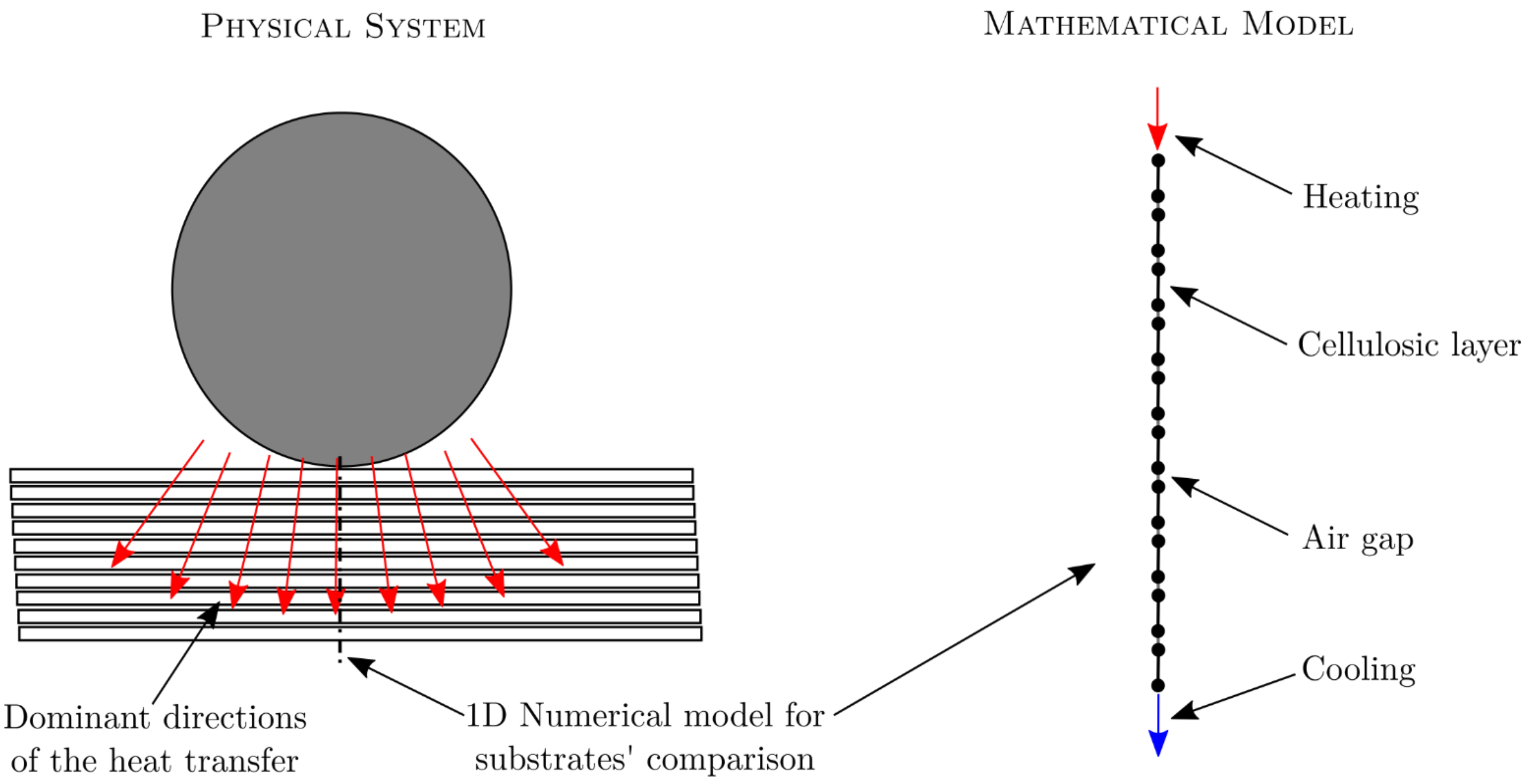




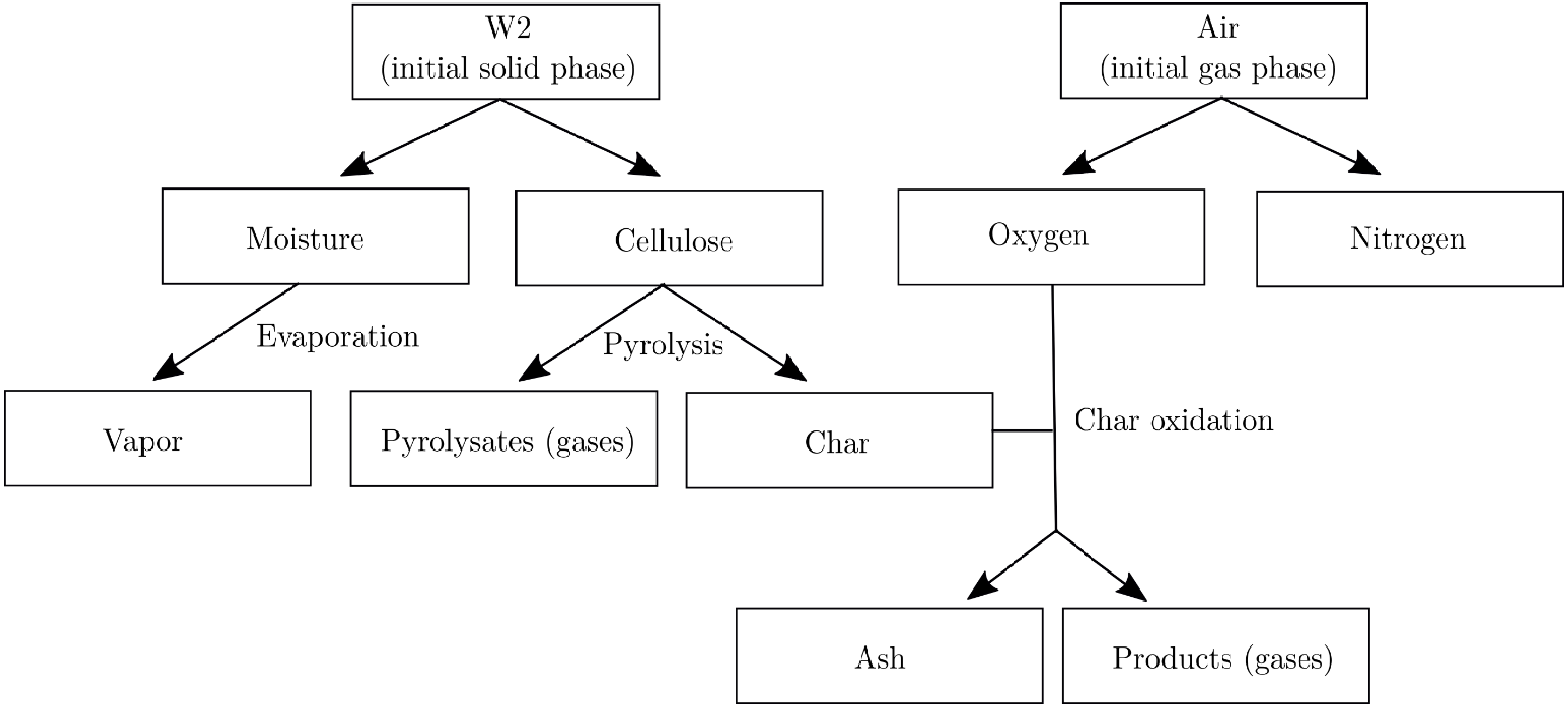
Case	Airgap min (mm)	Airgap max (mm)	Airgap av. (mm)
10 layers of W2 with LIP along tobacco column	0.021	0.060	0.041

Fraunhofer WKI

Modelling Approach



Scheme of the Thermal Degradation



Physical Equations and Material Data

Table 2 Reaction rates and heat sources of the model

Reaction	Expression
Moisture destruction	$\dot\omega'''_{d,m} = \bar\rho \cdot Y_m \cdot A_{ev} \cdot e^{-\frac{E_{ev}}{RT}}$
Vapor formation	$\dot\omega'''_{f,vap} = \dot\omega'''_{d,m}$
Cellulose destruction	$\dot\omega'''_{d,c} = \bar\rho \cdot Y_c \cdot A_{pyr} \cdot e^{-\frac{E_{pyr}}{RT}}$
Char formation	$\dot\omega'''_{f,ch} = \frac{\rho_{ch}}{\rho_c} \cdot \dot\omega'''_{d,c}$
Char destruction	$\dot\omega'''_{d,ch} = \bar\rho \cdot Y_{ch} \cdot A_{chox} \cdot e^{-\frac{E_{chox}}{RT}} \cdot Y_{O_2}$
Pyrolysates formation	$\dot\omega'''_{f,pg} = \left(1 - \frac{\rho_{ch}}{\rho_c}\right) \cdot \dot\omega'''_{d,c}$
Ash formation	$\dot\omega'''_{f,a} = \frac{\rho_a}{\rho_{ch}} \cdot \dot\omega'''_{d,ch}$
Oxygen destruction	$\dot\omega'''_{d,O_2} = \left(1 - \frac{\rho_a}{\rho_{ch}}\right) \cdot \dot\omega'''_{d,ch}$
End products formation	$\dot\omega'''_{f,pr} = 2 \cdot \left(1 - \frac{\rho_a}{\rho_{ch}}\right) \cdot \dot\omega'''_{d,ch} = 2 \cdot \dot\omega'''_{d,O_2}$
Total gas formation	$\dot\omega'''_{f,g} = \dot\omega'''_{f,vap} + \dot\omega'''_{f,pg} + \dot\omega'''_{f,pr} - \dot\omega'''_{d,O_2}$
Evaporation heat source	$\dot Q'''_{ev} = -\dot\omega'''_{d,m} \cdot \Delta H_{ev}$
Pyrolysis heat source	$\dot Q'''_{pyr} = -\dot\omega'''_{d,c} \cdot \Delta H_{pyr}$
Char oxidation heat source	$\dot Q'''_{chox} = -\dot\omega'''_{d,ch} \cdot \Delta H_{chox}$

Table 6 Material data

$\rho_c = 491.6kg/m^3$	$\rho_{s,c} = 1550kg/m^3$	$c_{p,c} = Eq.1J/kgK$	$k_c = 0.136W/mK$
$K_c = 7 \cdot 10^{-14}m^2$	$\varepsilon_c = 0.9$	$\rho_{ch} = 111kg/m^3$	$\rho_{s,ch} = 1500kg/m^3$
$c_{p,ch} = 1300J/kgK$	$k_{ch} = 0.105W/mK$	$K_{ch} = 1 \cdot 10^{-9}m^2$	$\varepsilon_{ch} = 0.95$
$\rho_a = 13kg/m^3$	$\rho_{s,a} = 1000kg/m^3$	$c_{p,a} = 1000J/kgK$	$k_a = 0.050W/mK$
$K_a = 1 \cdot 10^{-9}m^2$	$\varepsilon_a = 0.9$	$Y_m = 6.36\%$	$k_m = 0.58W/mK$
$c_{p,m} = 4181J/kgK$	$c_{p,g} = 1000J/kgK$	$M_{N_2} = 28g/mol$	$M_{O_2} = 32g/mol$
$M_{vap} = 18g/mol$	$M_{pg} = 50g/mol$	$M_{pr} = 40g/mol$	$A_{ev} = 5.13 \cdot 10^{10}1/s$
$E_{ev} = 88kJ/mol$	$\Delta H_{ev} = 2.44 \cdot 10^6 J/kg$	$A_{pyr} = 3.43 \cdot 10^{17}1/s$	$E_{pyr} = 225kJ/mol$
$\Delta H_{pyr} = 2.3 \cdot 10^5 J/kg$	$A_{chox} = 1 \cdot 10^8 1/s$	$E_{chox} = 140kJ/mol$	$\Delta H_{chox} = -2.5 \cdot 10^7 J/kg$
$\delta_{sb} = 0.19mm$	$\delta_{air} = 0.08mm$	$v_{cig} = 0.053mm/s$	$T_{cig} = Table4 \cdot \gamma_T$
$\gamma_T = 0.9$			

Table 3 Governing equations of the model

Governing Equation	Expression
Condensed mass conservation	$\frac{\partial\bar\rho}{\partial t} = -\dot\omega'''_{f,g}$
Gas phase mass conservation	$\frac{\partial(\rho_g \cdot \bar\Psi)}{\partial t} + \frac{\partial \dot m''}{\partial z} = \dot\omega'''_{f,g}$
Condensed species conservation	$\frac{\partial(\bar\rho \cdot Y_i)}{\partial t} = \dot\omega'''_{f,i} - \dot\omega'''_{d,i}$
Gas species conservation	$\frac{\partial(\rho_g \cdot \bar\Psi \cdot Y_j)}{\partial t} + \frac{\partial(\dot m'' \cdot Y_j)}{\partial z} = -\frac{\partial \dot j''_j}{\partial z} + \dot\omega'''_{f,j} - \dot\omega'''_{d,j}$
Energy conservation	$\frac{\partial(\bar\rho \cdot \bar h)}{\partial t} = -\frac{\partial \dot q''}{\partial z} - \dot m'' \cdot c_{p,g} \cdot \frac{\partial T}{\partial z} + \sum_{k=1}^{3} \dot Q'''_k + \sum_{i=1}^{4} \left(\dot\omega'''_{f,i} - \dot\omega'''_{d,i}\right) \cdot h_i$
Momentum conservation	$\frac{\partial}{\partial t}\left(\frac{P\bar M}{RT} \cdot \bar\Psi\right) = \frac{\partial}{\partial z}\left(\frac{\bar K}{\nu} \cdot \frac{\partial P}{\partial z}\right) + \dot\omega'''_{f,g} - g \cdot \frac{\partial}{\partial z}\left(\frac{\bar K}{\nu}\rho_g\right)$

Table 5 Computation of the material properties. Note the superscript ¯ indicates average property, $T_d = 200K$, $T_r = 298K$ and D is calculated via Chapman-Enskog theory.

$X_i = \bar\rho \frac{Y_i}{\rho_i}$	$\bar\rho = \left(\sum_{i=1}^{4} \frac{Y_i}{\rho_i}\right)^{-1}$	$\bar\Psi = \sum_{i=1}^{4} X_i \Psi_i$	$\Psi_i = 1 - \frac{\rho_i}{\rho_{s,i}}$
$\bar k = \sum_{i=1}^{4} X_i k_i$	$\bar{c_p} = \sum_{i=1}^{4} Y_i c_{p,i}$	$\bar h = \sum_{i=1}^{4} Y_i h_i$	$h_i = \frac{c_{p,i,25^oC}}{n_{c_{p,i}}}\left(T\left(\frac{T}{Tr}\right)^{n_{c_{p,i}}} - T_d\left(\frac{T_d}{Tr}\right)^{n_{c_{p,i}}}\right)$
$\bar\varepsilon = \sum_{i=1}^{4} X_i \varepsilon_i$	$\bar K = \sum_{i=1}^{4} X_i K_i$	$\bar M = \sum_{j=1}^{4} X_j M_j$	$\rho_g = \frac{P\bar M}{RT}$
$c_{p,g} = c_{p,j}$	$\bar h_g = c_{p,g}(T - Td)$	$k_g = c_{p,g}\rho_g D$	$\nu = D$

Boundary Conditions

$$-k\frac{\partial T}{\partial z}\Big|_{u} = -\bar{\varepsilon}\sigma\left(T^4|_u - T_{cig}^4\right) - h_{cs}\left(T|_u - T_{cig}\right)$$

Where *Tcig* was obtained from the temperatures reported by Baker and reduced by a factor of 0.9

Burning section distance (mm)	Time (s)	Temperature (K)
0.0	0	298
1.0	19	347
2.0	38	400
3.0	57	592
4.0	75	763
5.0	94	788
6.0	113	787
7.0	132	760
8.0	151	730
9.0	170	678
10.0	189	643
11.0	208	614
12.0	226	572
12.7	240	298
14.0	264	298

$$-k\frac{\partial T}{\partial z}\Big|_{l} = -\bar{\varepsilon}\sigma\left(T^4|_l - T_{amb}^4\right) - h_{sa}\left(T|_l - T_{amb}\right)$$

Numerical Implementation

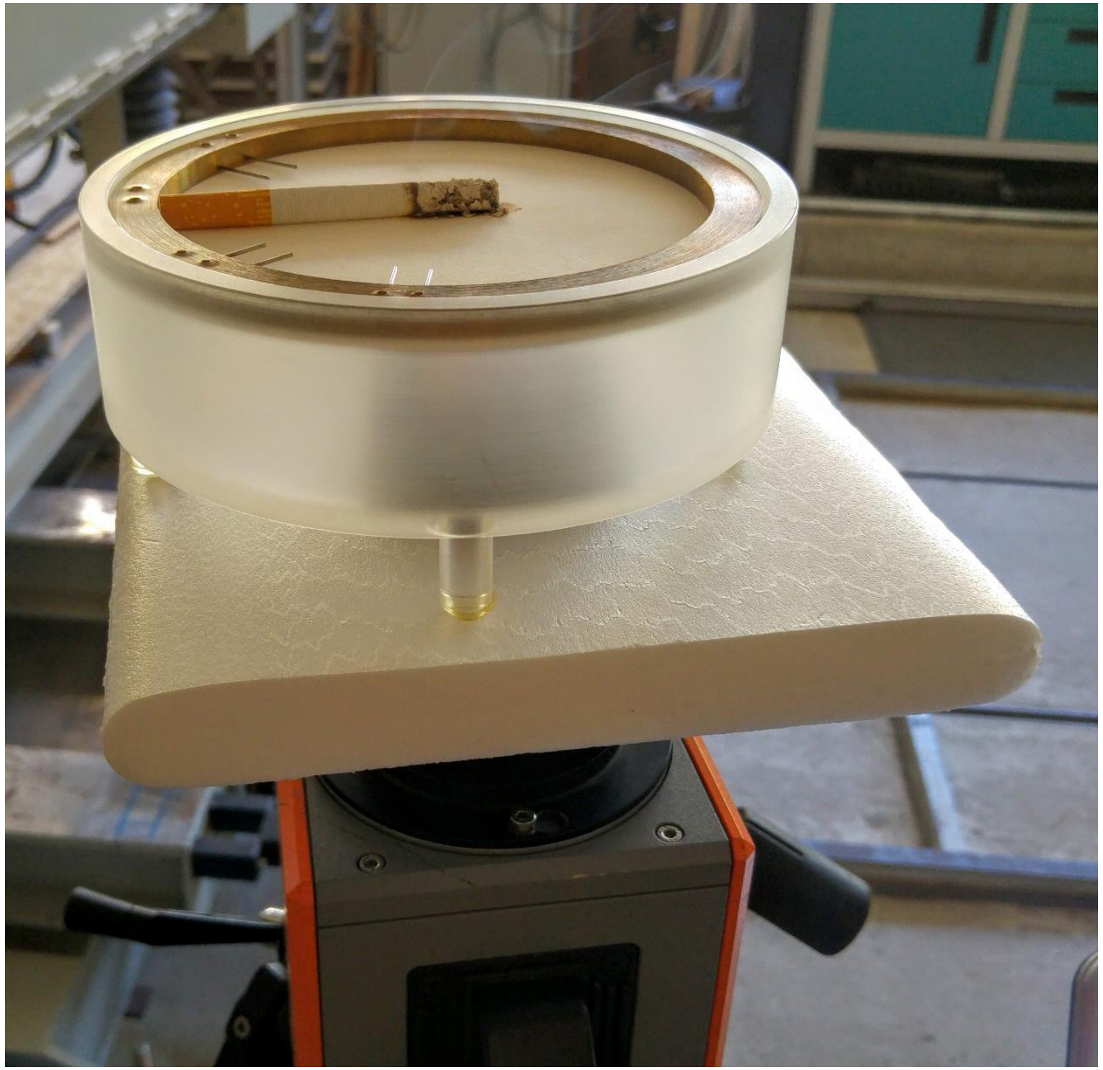
- Air gap modelled as a non-charring material with temperature dependent properties

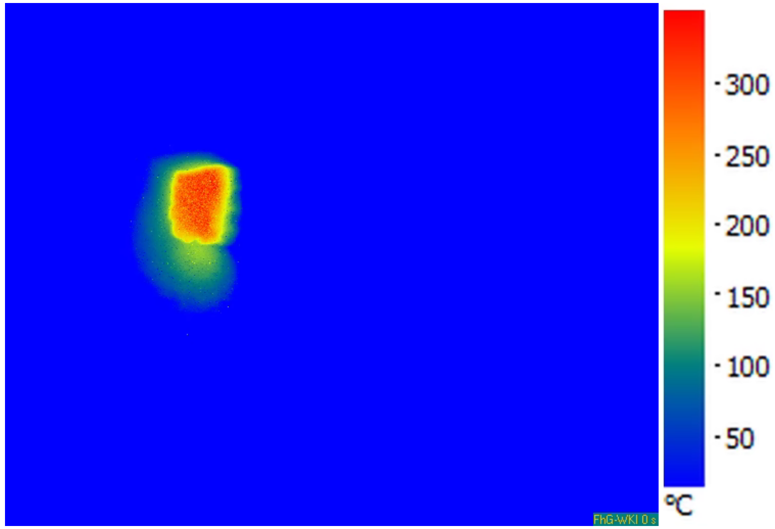
- Mesh size of 2 μm (1311 elements) and time step 0.01 seconds, tolerance x $1 \cdot 10^{-4}$

- Resolution via Finite Volume Method (FVM), implicit scheme, tridiagonal matrix algorithm.

- CFD Model implemented in the research software Gpyro (created at the University of California at Berkeley under the sponsorship of the NASA).

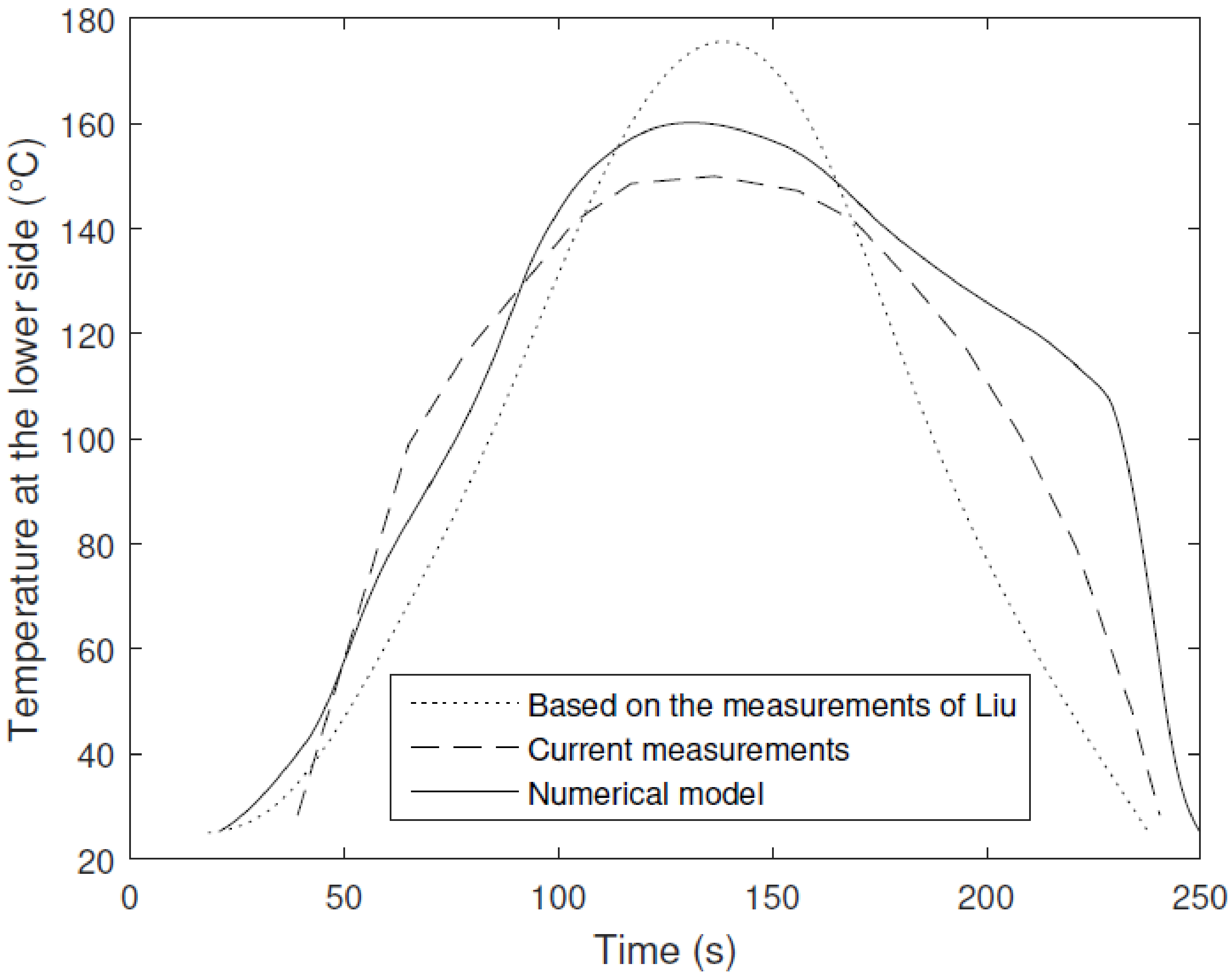
Model Validation: Experiments





Fraunhofer WKI

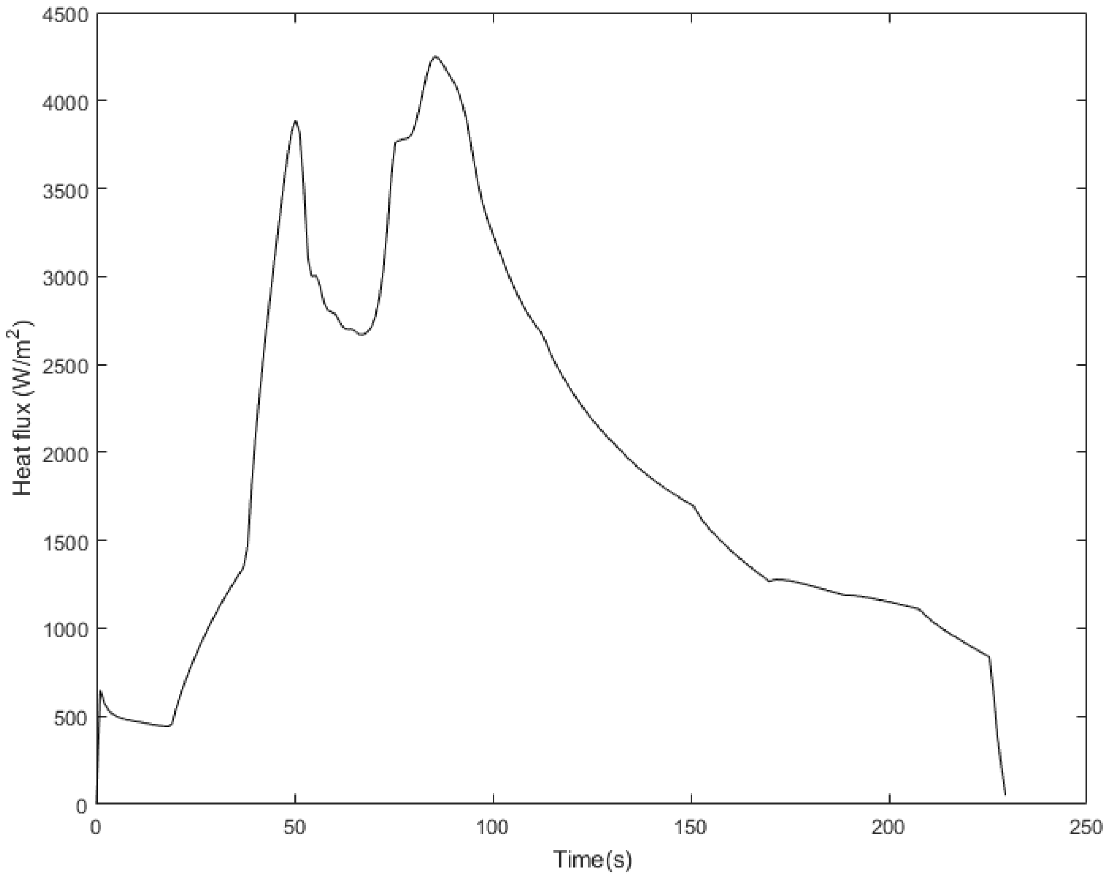
Model Validation: Comparison



Fraunhofer WKI

Detailed Analysis: Reference Parameter

- Absorbed heat flux function is an adequate reference for analysis and comparison purposes



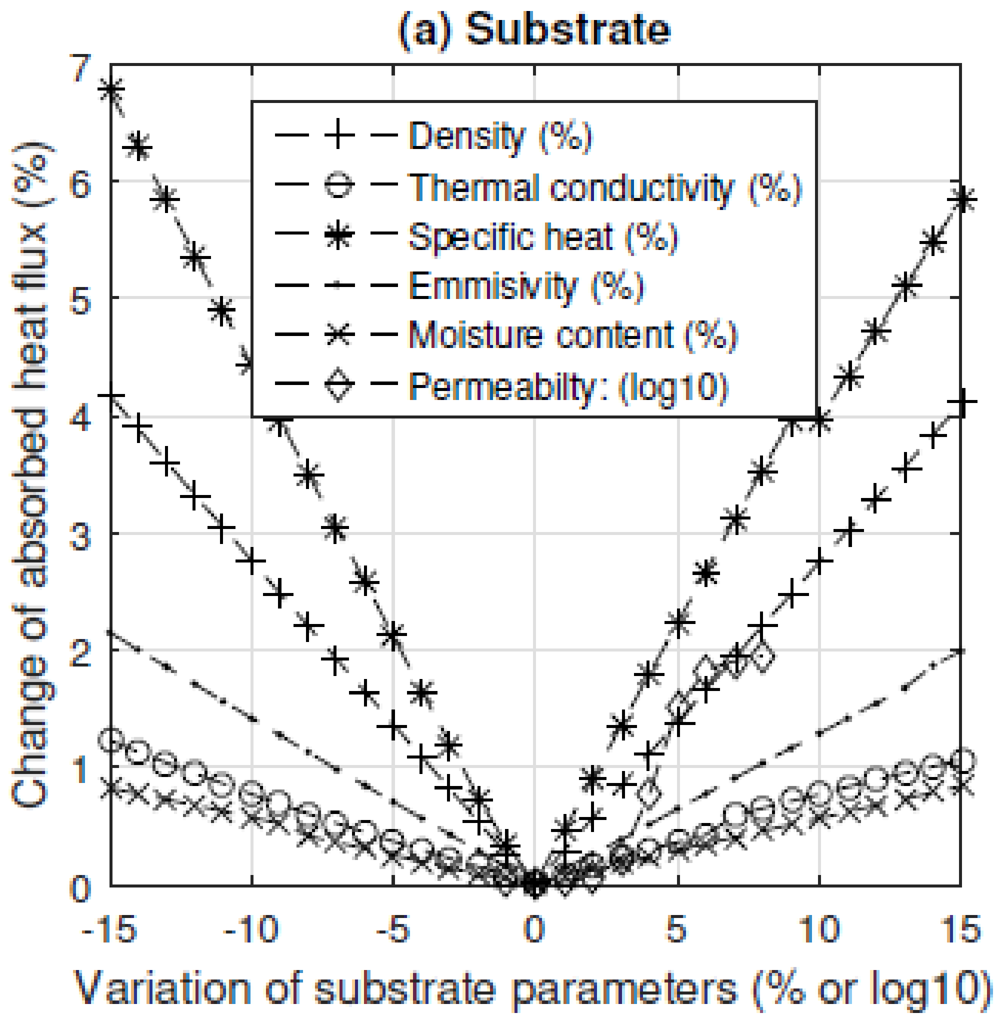
$$\dot{q}''_{in} = \bar{\varepsilon}\sigma\left(T_{cig}^{4} - T^{4}|_{u}\right) + h_{cs}\left(T_{cig} - T|_{u}\right)$$

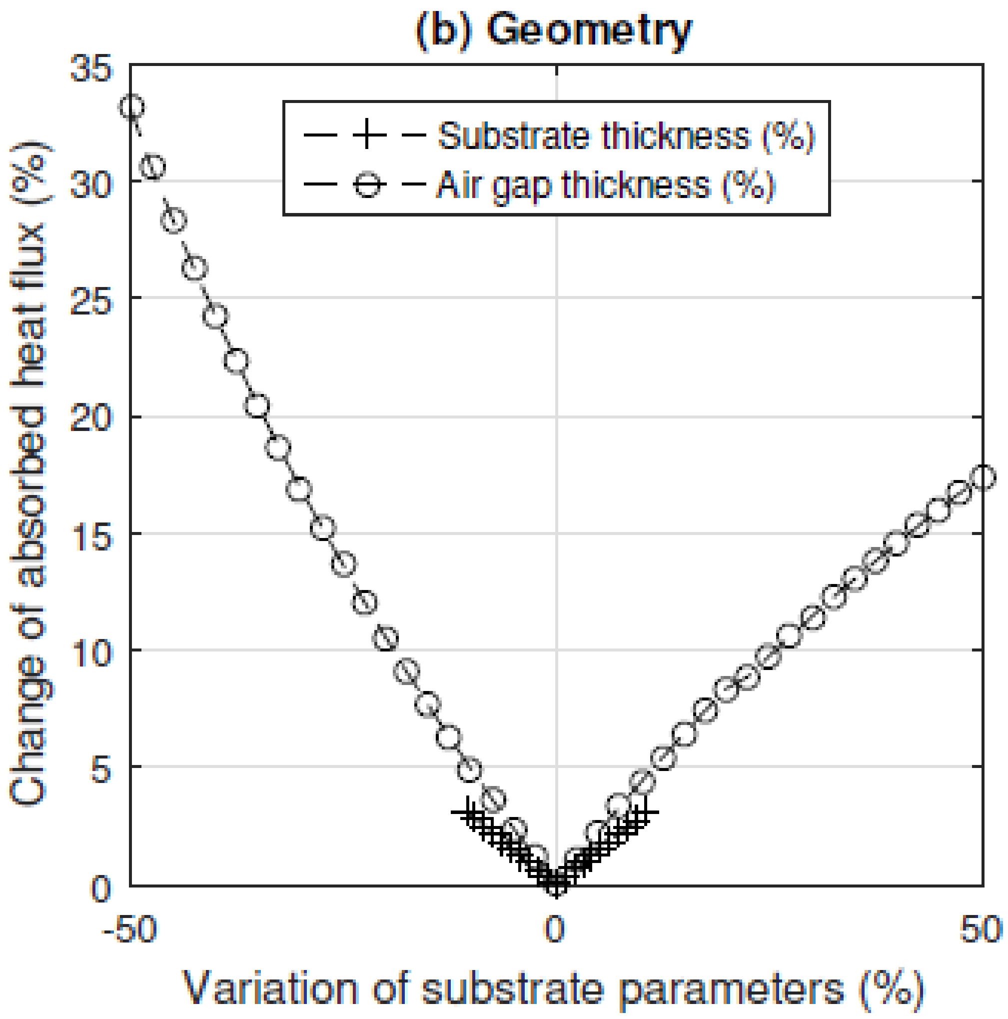
$$\Delta\dot{q}''_{in} = \frac{|\dot{q}''_{in}(t) - \dot{q}''_{in,r}(t)|}{\dot{q}''_{in,r}(t)} \cdot 100$$

Fraunhofer
WKI

Detailed Analysis: Parametric Study I

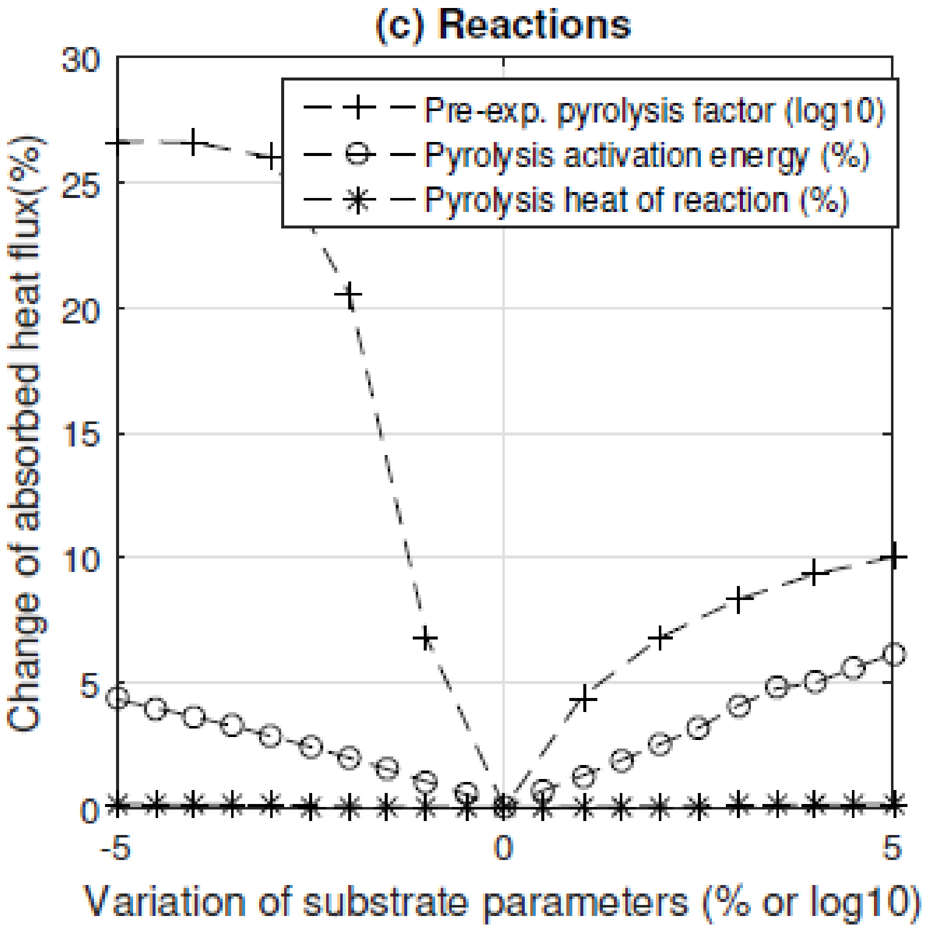
- After 363 IP Simulations…

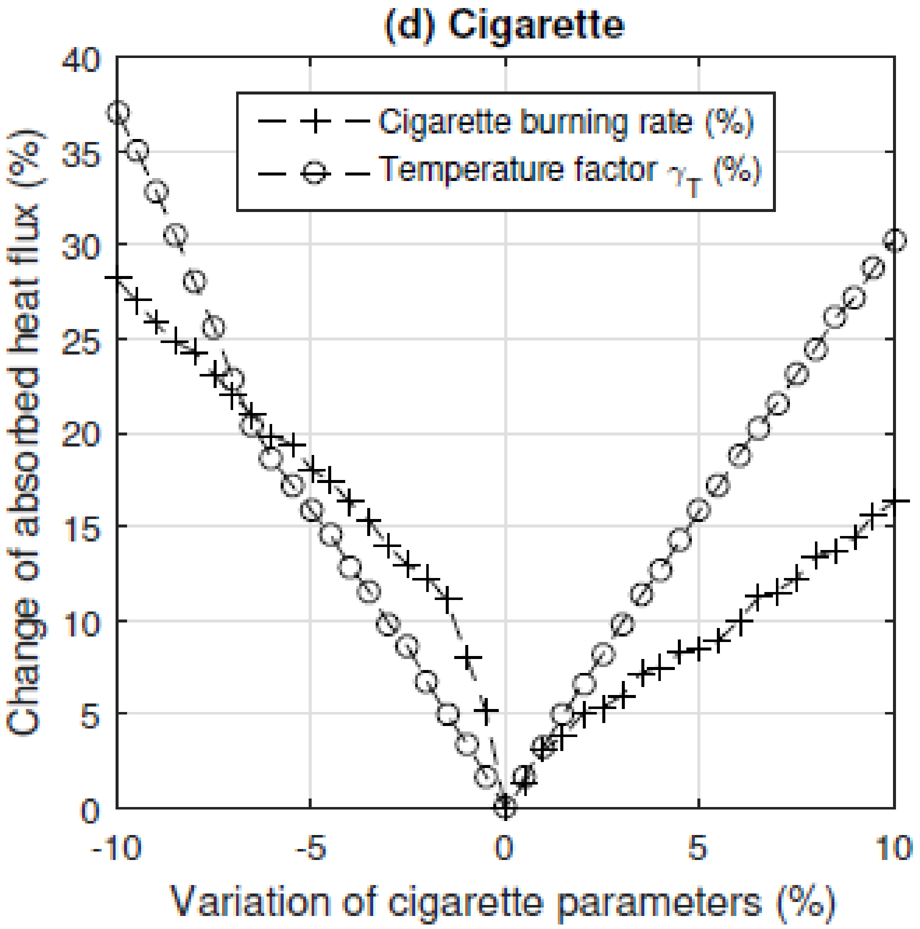




Detailed Analysis: Parametric Study II

- After 363 IP Simulations…





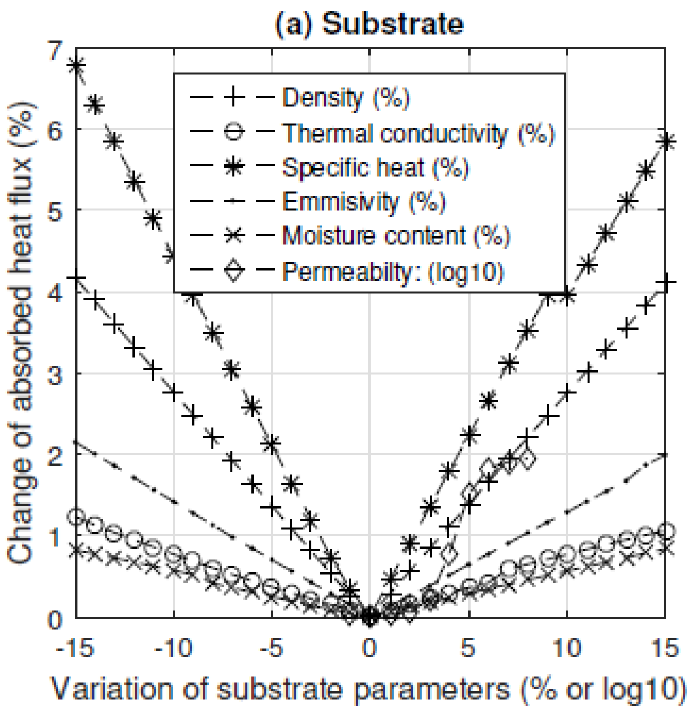
Fraunhofer WKI

Detailed Analysis: Potential Influence of the Substrate

- Now it is possible to state whether the substrate may have an influence or not…

Property	Method	No. of tests	Mean (±SD)
Paper thickness (μm)	ISO 534 [7]	20	191 ± 7
Air layer thickness (μm)	Laser triangulation	1	80
Paper density (g/m^3)	ISO 534 [7]	20	0.525 ± 0.021
Moisture content (%)	ISO 287 [6]	20	6.360 ± 0.078
Char mass fraction (1)	TGA+SCE	9	0.21
Ash mass fraction (1)	TGA+SCE	9	0.02
Specific volume (m^3/g)	ISO 534 [7]	20	1.909 ± 0.078
Grammage (g/m^2)	ISO 536 [8]	20	99.915 ± 0.92
Permeance (μm/Pa·s)	ISO 5636-3 [9]	10	25.7 ± 1.14
Permeability (m^2)	Calculated from permeance	10	$7.29 \cdot 10^{-14}$
Thermal conductivity (W/mK)	THB	8	0.164 ± 0.011
Heat capacity (J/kgK)	DSC	4	Eq. 1
Pre-exponential factor of pyrolysis (s^{-1})	TGA+SCE	9	$3.4 \cdot 10^{17}$
Activation energy of pyrolysis (kJ/mol)	TGA+SCE	9	225
Heat of the pyrolysis (kJ/kg)	DSC	4	230
Pre-exponential factor of char oxidation (s^{-1})	TGA+SCE	9	$1 \cdot 10^{8}$
Activation energy of char oxidation (kJ/mol)	TGA+SCE	9	140
Heat of char oxidation (kJ/kg)	DSC/Literature [11]	-	$-25 \cdot 10^{3}$
Gross heat of combustion (kJ/kg)	ISO 1716 [5]	1 (500g)	16808
Net heat of combustion (kJ/kg)	ISO 1716 [5]	1 (500g)	15432
Roughness at the upper (A) and lower (B) sides (ml/min)	ISO 8791-2 [10]	10	A=1685 ± 88.4 B=1165 ± 41.2
Elemental analysis (%)	IRMS	3	C = 42.906 ± 0.043 H = 6.465 ± 0.040 N = 2.829 ± 0.462 S = 0.303 ± 0.071

Potential influence

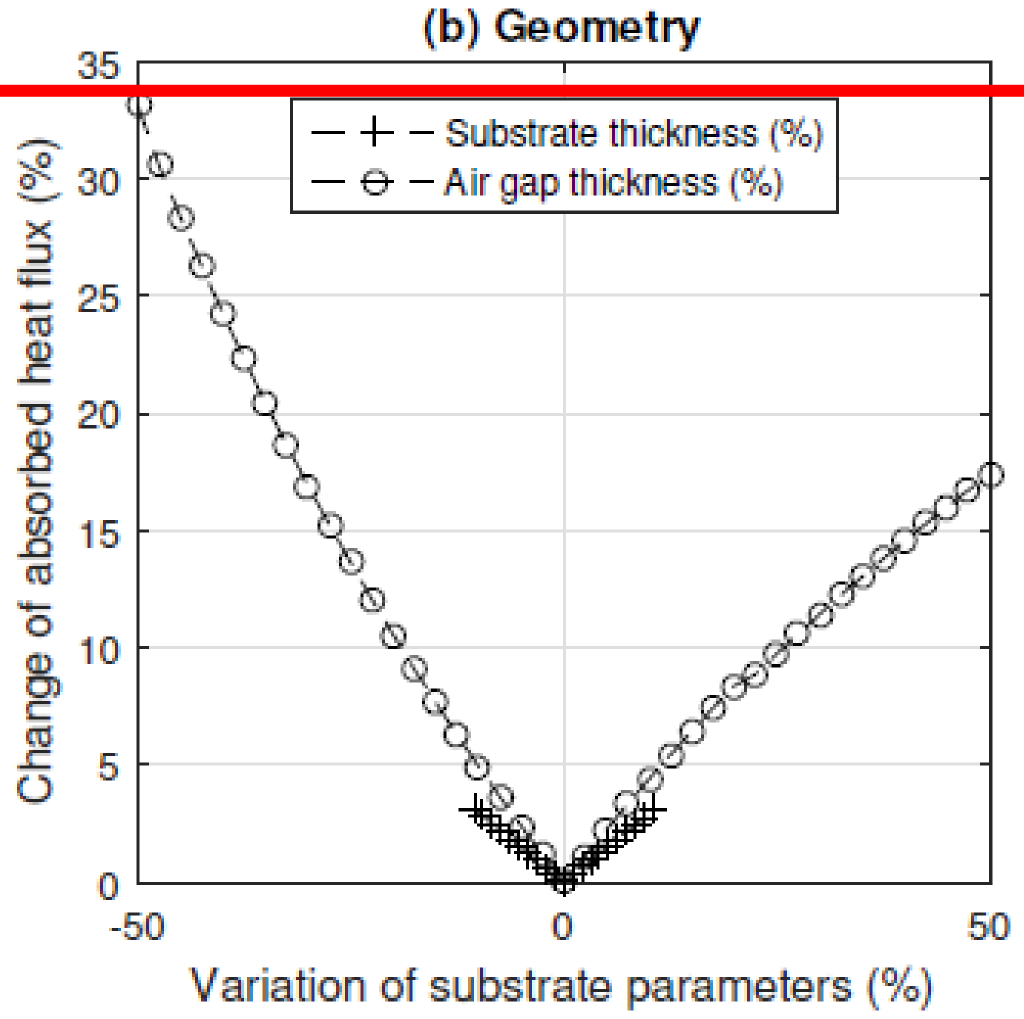


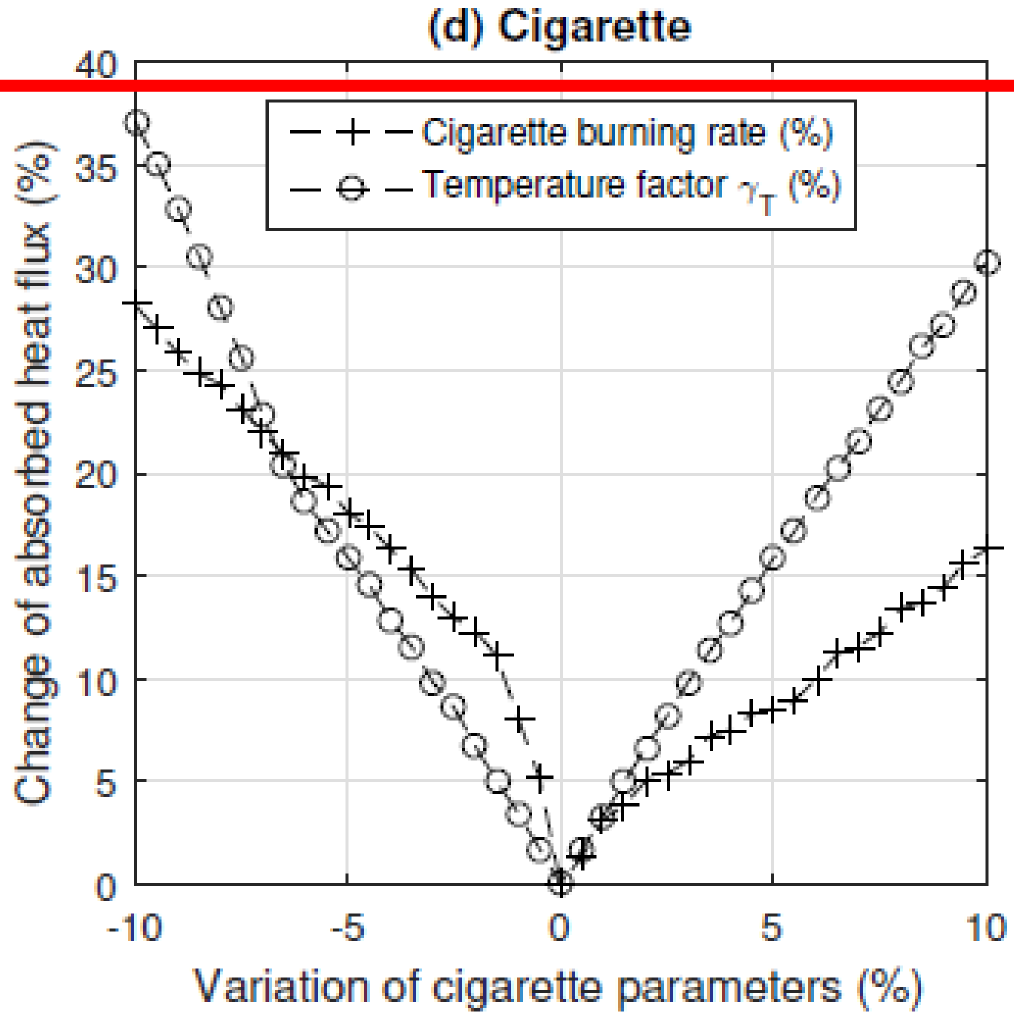
Measured variation

Detailed Analysis: Summary

Source of Variability	Range of Variability	Expected effect on heat absorbed during IP testing
Thermophysical properties of substrate	About 7% according to measurements	Below 3%
Chemical kinetics	Not possible to ascertain (best fit)	Could be significant if variability on activation energy
Geometry	50% (on air gap) according to measurements	About 33%
Cigarette (only temperature and burning rate)	10% (estimated)	About 35%

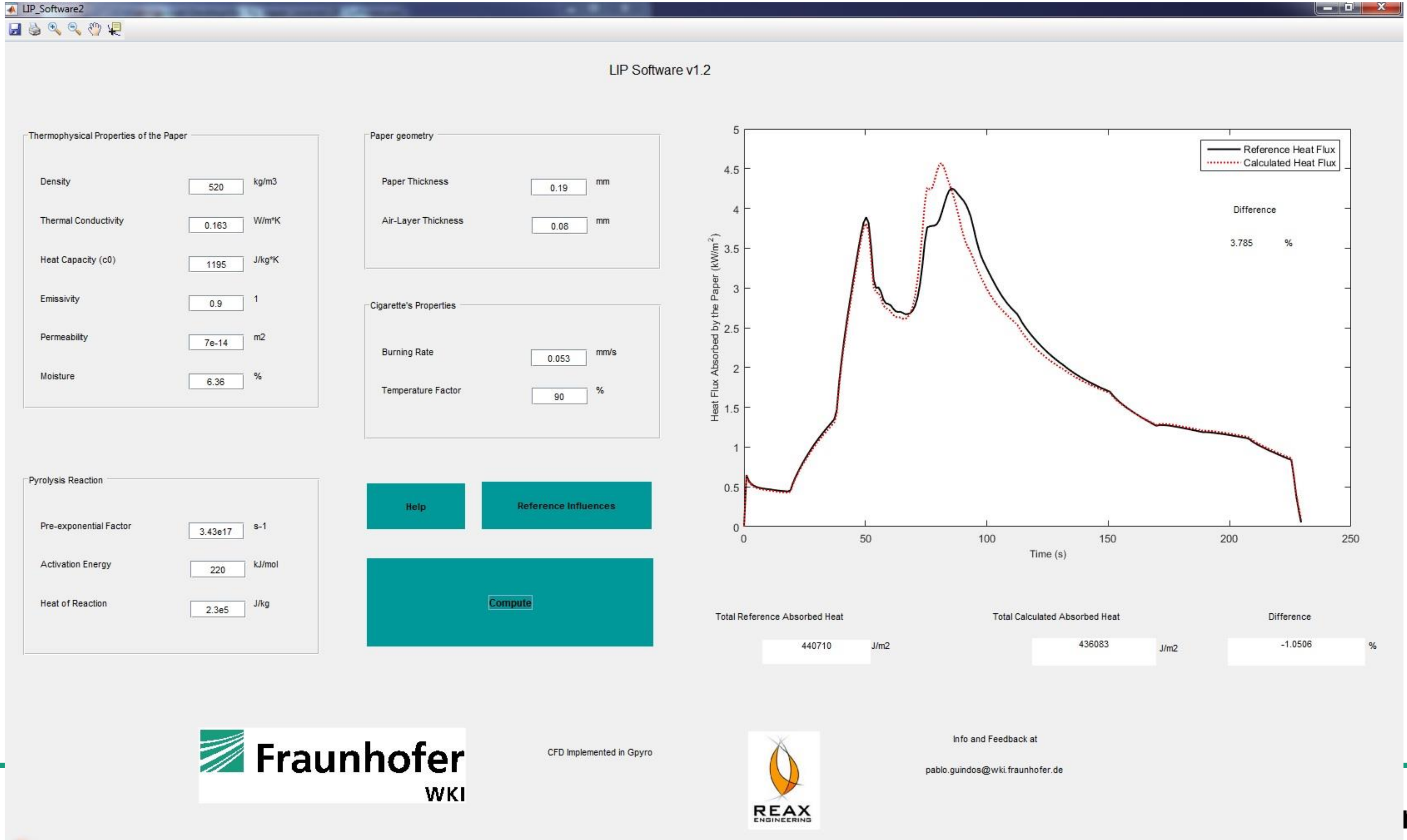
Detailed Analysis: Comparison with Cigarette





SIMULIP Software

- For the non simulated cases…



Conclusions

- Thermodynamic characterization as expected except that air gap is very large and variable
- A CFD model was created and successfully simulated the substrate during IP testing
- According to the model:
  - Most influencing parameters: Heat Capacity, Activation Energy, Air Gap, Temperature and Burning Rate of the Cigarette.
  - Influence of air gap compares to that expected for the cigarette.
  - Accordingly, not only the cigarette but also the substrate could be responsible of the poor repeatability of the test.
- A software called SIMULIP was developed and could be used for future IP development.

THANKS FOR YOUR ATTENTION!

Dr. Pablo Guindos
pablo.guindos@wki.fraunhofer.de