IRSN
INSTITUT
DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

Approche préliminaire pour la modélisation de la pyrolyse dans le code ISIS

G. Boyer, A. Kacem, S. Suard

IRSN/PSN-RES/SA2I/LIE

GDR, Bourges, 29/1/2015

Outline

Outline

Reasons for the raise of generalized pyrolysis modellings

Considered fire sources

- Liquids

Reasons for the raise of generalized pyrolysis modellings

Considered fire sources

- Liquids
- Homogeneous materials: semi-transparent polymers in Glove Boxes. . .

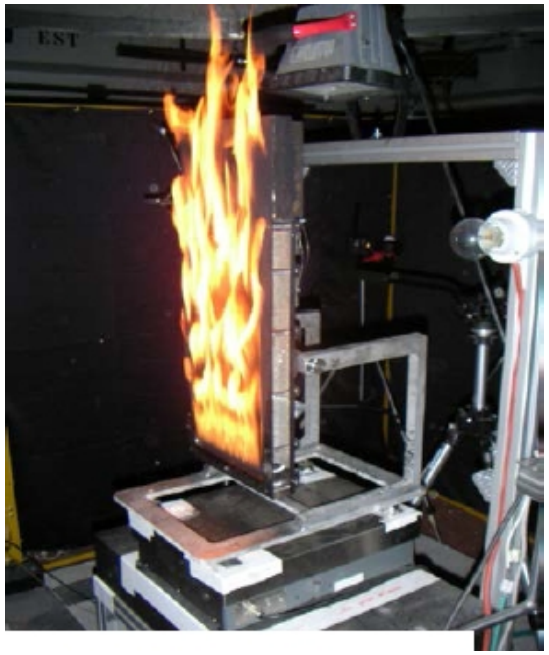


Figure : Flaming vertical PMMA flat plate

Reasons for the raise of generalized pyrolysis modellings

Considered fire sources

- Liquids
- Homogeneous materials: semi-transparent polymers in Glove Boxes...
- Charring materials in cables...

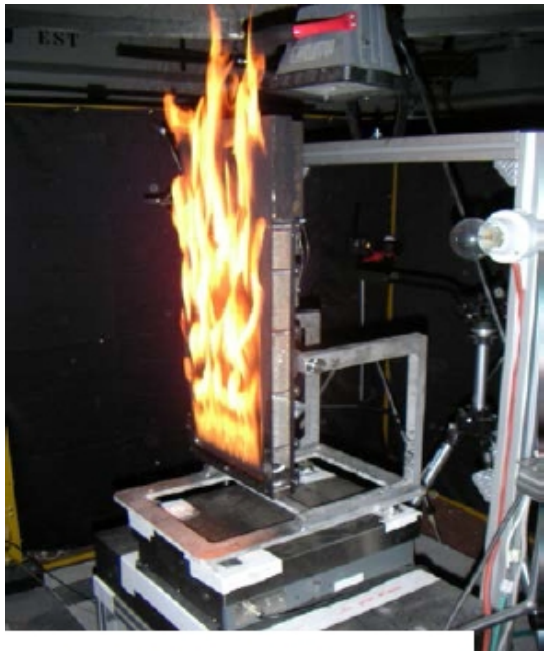


Figure : Flaming vertical PMMA flat plate

Reasons for the raise of generalized pyrolysis modellings

Considered fire sources

- Liquids
- Homogeneous materials: semi-transparent polymers in Glove Boxes...
- Charring materials in cables...
- Complex solids...

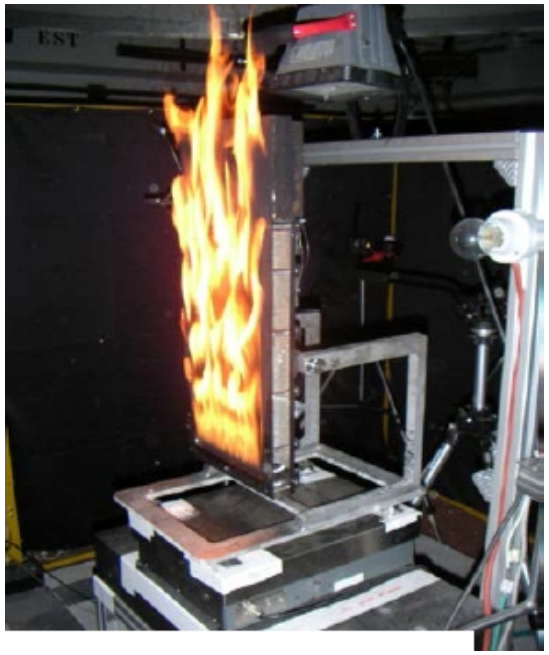


Figure : Flaming vertical PMMA flat plate

Figure : Cable tray fire

Pyrolysis modelling: a multiphysic phenomenon

Heat transfer

- Conduction, internal radiation, internal convection in porous media
- Fluid-solid interface: turbulent surface heat transfer, radiation
- Classic heat conservation laws adapted to multiphasic/heterogeneous flows

Mass transfer and volume conservation

- Solid mass loss due to the degradation reactions
- Pyrolysis volatiles generation
- Solid volume evolution: erosion, intumescence
- Classic multicomponent mass conservation laws

Thermochemistry

- Complex solid fire sources to be modeled by multi-species pyrolysis:
- Material degradation
  - degradation scenarios
  - thermokinetic aspects: Arrhenius constants, species concentration dependence
  - Influence of the O_2 concentration
- No theoretical background, empirical approach

Consequences on the materials pyrolysis characterization

Engineering approach vs. fundamental chemistry

- Fundamental chemistry:
  - molecular description of the materials degradation
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - Out of reach in CFD

Consequences on the materials pyrolysis characterization

Engineering approach vs. fundamental chemistry

- Fundamental chemistry:
  - molecular description of the materials degradation
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - Out of reach in CFD
- Applied chemistry
  - complex, empirical degradation scenarii
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - model-free constants, predictive aspects
  - exhaustive materials characterizations in nuclear safety out of reach
  - Need for complete, accurate models

Consequences on the materials pyrolysis characterization

Engineering approach vs. fundamental chemistry

- Fundamental chemistry:
  - molecular description of the materials degradation
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - Out of reach in CFD
- Applied chemistry
  - complex, empirical degradation scenarii
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - model-free constants, predictive aspects
  - exhaustive materials characterizations in nuclear safety out of reach
  - Need for complete, accurate models
- Engineering approach
  - one material $\leftrightarrow$ one (or a few) reactions
  - available parameters: "robust" values
  - unknown parameters determined by inverse methods
  - Model-dependent constants
  - Constants relevance ? (Ghorbani et al., 2013)
  - Ability to consider partly characterized materials

Consequences on the materials pyrolysis characterization

Engineering approach vs. fundamental chemistry

- Fundamental chemistry:
  - molecular description of the materials degradation
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - Out of reach in CFD
- Applied chemistry
  - complex, empirical degradation scenarii
  - accurate characterization of the thermal, radiative, geometrical materials properties
  - model-free constants, predictive aspects
  - exhaustive materials characterizations in nuclear safety out of reach
  - Need for complete, accurate models
- Engineering approach
  - one material $\leftrightarrow$ one (or a few) reactions
  - available parameters: "robust" values
  - unknown parameters determined by inverse methods
  - Model-dependent constants
  - Constants relevance ? (Ghorbani et al., 2013)
  - Ability to consider partly characterized materials

Worth enhancing basic pyrolysis modellings and material characterizations for CFD computations ?

Outline

Pyrolysis modelling: minimal considered phenomena

Heat transfer

- Conduction, internal radiation, internal convection in porous media
- Fluid-solid interface: turbulent surface heat transfer, radiation

Mass transfer and volume conservation

- Solid mass loss due to the degradation reactions
- Pyrolysis volatiles generation
- Solid volume evolution: erosion, intumescence

Thermochemistry

- Complex sources to be modeled by multi-species pyrolysis:
- Material degradation
  - degradation path: comptetitive and sequential reactions
  - thermokinetic aspects: Arrhenius laws with species concentration dependence
  - Influence of the O_2 concentration

Pyrolysis modelling: minimal considered phenomena

Heat transfer

- **1D**-Conduction, internal radiation, internal convection in porous media
- Fluid-solid interface: **simplified convective surface heat transfer**, radiation

Mass transfer and volume conservation

- Solid mass loss due to the degradation reactions
- Pyrolysis volatiles generation
- Solid volume evolution: erosion, intumescence — **ALE method**

Thermochemistry

- Complex sources to be modeled by multi-species pyrolysis:
  - N_S materials/solid chemical species
  - N_G pyrolysis volatiles
- Material degradation
  - degradation path: N_R comptetitive and sequential reactions
  - thermokinetic aspects: Arrhenius laws with species concentration dependence
  - Influence of the O_2 concentration

Monophasic pyrolysis modelling: main features

- Test implementation in a separate software
  - CFD and pyrolysis are decoupled
  - preliminary tests of various schemes and modellings implementations
  - easy use of optimization techniques for parameters evaluation

Monophasic pyrolysis modelling: main features

- Test implementation in a separate software
  - CFD and pyrolysis are decoupled
  - preliminary tests of various schemes and modellings implementations
  - easy use of optimization techniques for parameters evaluation
- Special care for stability and consistency criteria
  - Pseudo-transport equations writen in conservative form (Kuo, 1986)
  - finite volume space discretization
  - backward Euler implicit time integration

Monophasic pyrolysis modelling: main features

- Test implementation in a separate software
  - CFD and pyrolysis are decoupled
  - preliminary tests of various schemes and modellings implementations
  - easy use of optimization techniques for parameters evaluation
- Special care for stability and consistency criteria
  - Pseudo-transport equations writen in conservative form (Kuo, 1986)
  - finite volume space discretization
  - backward Euler implicit time integration
- Solved equations
  - Enthalpy conservation; variable: T (temperature)
  - Solid mass conservation; variables: solid partial densities ($\rho_{S,j}$)
  - Volume conservation; variable: solid deformation velocity ($\mathbf{u}_{e,S}$)

Monophasic pyrolysis modelling: main features

- Test implementation in a separate software
  - CFD and pyrolysis are decoupled
  - preliminary tests of various schemes and modellings implementations
  - easy use of optimization techniques for parameters evaluation
- Special care for stability and consistency criteria
  - Pseudo-transport equations writen in conservative form (Kuo, 1986)
  - finite volume space discretization
  - backward Euler implicit time integration
- Solved equations
  - Enthalpy conservation; variable: T (temperature)
  - Solid mass conservation; variables: solid partial densities ($\rho_{S,j}$)
  - Volume conservation; variable: solid deformation velocity ($\mathbf{u}_{e,S}$)
- Considered parameters
  - Arrhénius constants: $A_{s,j}$, $E_{a,i}$
  - reaction orders: $n_{R,i}$
  - heat of pyrolysis: L_i
  - phasic densities: $\rho^0_{S,j}$
  - Thermal parameters: $c_{p,S,j}$, $\lambda_{S,j}$, $\kappa_{S,j}$ (heat capacities, conduction, radiative absorption)
  - Interface parameters: h (convective heat exchange coefficient), ε (surface emissivity)
  - gas phase parameters: $\rho_{G,j}$, $c_{p,G,j}$ (partial densities, heat capacities)

Diphasic pyrolysis modelling: main features

- Test implementation in a separate software
  - CFD and pyrolysis are decoupled
  - preliminary tests of various schemes and modellings implementations
  - easy use of optimization techniques for parameters evaluation
- Special care for stability and consistency criteria
  - Pseudo-transport equations writen in conservative form (Kuo, 1986)
  - finite volume space discretization
  - backward Euler implicit time integration
- Solved equations
  - Enthalpy conservation; variable: T (temperature)
  - Solid mass conservation; variables: solid partial densities ($\rho_{S,j}$)
  - Volume conservation; variable: solid deformation velocity ($\mathbf{u}_{e,S}$)
  - Gaseous mass conservation ($\rho_G, p_G, \mathbf{u}_{e,G}$)
  - Gaseous species conservation ($Y_{G,j}$)
- Considered parameters
  - Arrhénius constants: $A_{s,j}, E_{a,i}$
  - reaction orders: $n_{R,i}$
  - heat of pyrolysis: L_i
  - phasic densities: $\rho^0_{S,j}$
  - Thermal parameters: $c_{p,S,j}, \lambda_{S,j}, \kappa_{S,j}$ (heat capacities, conduction, radiative absorption)
  - Interface parameters: h (convective heat exchange coefficient), ε (surface emissivity)
  - gas phase parameters: $\rho_{G,j}, c_{p,G,j}$ (partial densities, heat capacities)
  - Porosity parameters : ϕ, K, μ (porosity, permeability, viscosity)

Outline

Principle of the current validation: case of PMMA

- Comparison to calorimeter cone experiments by Kashiwagi and Ohlemiller, 1982
  - non-flaming configurations
  - imposed radiative heat flux: $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2
  - Oxydative and **non-oxydative** conditions

Principle of the current validation: case of PMMA

- Comparison to calorimeter cone experiments by Kashiwagi and Ohlemiller, 1982
  - non-flaming configurations
  - imposed radiative heat flux: $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2
  - Oxydative and **non-oxydative** conditions
- Assumed degradation path in non-oxydative conditions:

$$\underbrace{\text{PMMA}}_{\text{solid}} \rightarrow \underbrace{\text{bPMMA}}_{\text{solid, bubbled}} \; ; \quad \text{bPMMA} \rightarrow \underbrace{\text{MMA}}_{\text{volatile}}$$

Principle of the current validation: case of PMMA

- Comparison to calorimeter cone experiments by Kashiwagi and Ohlemiller, 1982
  - non-flaming configurations
  - imposed radiative heat flux: $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2
  - Oxydative and **non-oxydative** conditions
- Assumed degradation path in non-oxydative conditions:

$$\underbrace{\text{PMMA}}_{\text{solid}} \rightarrow \underbrace{\text{bPMMA}}_{\text{solid, bubbled}} \; ; \quad \text{bPMMA} \rightarrow \underbrace{\text{MMA}}_{\text{volatile}}$$

- Widespread physical parameters found in the litterature (Bal and Rein, 2013) !
  - $\rho_S^0 \approx 1100$ kg/m^3
  - $\lambda_S \in [0.13, 0.27]$ W/m/K, $c_{p,S} \in [1200, 3050]$ J/kg/K
  - $\kappa_S \in [333, 5430]$ m^{-1}, $\varepsilon \in [0.85, 1]$
  - Arrhenius constants: $A_S \in [1, 10^{23}]$ s^{-1}, $E_a \in [3.1\ 10^4, 2.9\ 10^5]$ J/mol, $n_R \in [0.5, 2.2]$
  - Heat of pyrolysis: $L \in [4.2\ 10^5, 10^6]$ J/kg ... in non-conservative modellings !

Principle of the current validation: case of PMMA

- Comparison to calorimeter cone experiments by Kashiwagi and Ohlemiller, 1982
  - non-flaming configurations
  - imposed radiative heat flux: $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2
  - Oxydative and **non-oxydative** conditions
- Assumed degradation path in non-oxydative conditions:

$$\underbrace{\text{PMMA}}_{\text{solid}} \rightarrow \underbrace{\text{bPMMA}}_{\text{solid, bubbled}} \; ; \quad \text{bPMMA} \rightarrow \underbrace{\text{MMA}}_{\text{volatile}}$$

- Widespread physical parameters found in the litterature (Bal and Rein, 2013) !
  - $\rho_S^0 \approx 1100$ kg/m^3
  - $\lambda_S \in [0.13, 0.27]$ W/m/K, $c_{p,S} \in [1200, 3050]$ J/kg/K
  - $\kappa_S \in [333, 5430]$ m^{-1}, $\varepsilon \in [0.85, 1]$
  - Arrhenius constants: $A_S \in [1, 10^{23}]$ s^{-1}, $E_a \in [3.1\ 10^4, 2.9\ 10^5]$ J/mol, $n_R \in [0.5, 2.2]$
  - Heat of pyrolysis: $L \in [4.2\ 10^5, 10^6]$ J/kg ... in non-conservative modellings !
- Convective heat transfer coefficient
  - $h \in [3.5, 34]$ W/m^2/K
  - Depends on the flow turbulence struture at the interface: constant value in any conditions ?

Principle of the current validation: case of PMMA

- Comparison to calorimeter cone experiments by Kashiwagi and Ohlemiller, 1982
  - non-flaming configurations
  - imposed radiative heat flux: $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2
  - Oxydative and **non-oxydative** conditions
- Assumed degradation path in non-oxydative conditions:

$$\underbrace{\text{PMMA}}_{\text{solid}} \rightarrow \underbrace{\text{bPMMA}}_{\text{solid, bubbled}} \; ; \quad \text{bPMMA} \rightarrow \underbrace{\text{MMA}}_{\text{volatile}}$$

- Widespread physical parameters found in the litterature (Bal and Rein, 2013) !
  - $\rho_S^0 \approx 1100$ kg/m^3
  - $\lambda_S \in [0.13, 0.27]$ W/m/K, $c_{p,S} \in [1200, 3050]$ J/kg/K
  - $\kappa_S \in [333, 5430]$ m^{-1}, $\varepsilon \in [0.85, 1]$
  - Arrhenius constants: $A_S \in [1, 10^{23}]$ s^{-1}, $E_a \in [3.1\ 10^4, 2.9\ 10^5]$ J/mol, $n_R \in [0.5, 2.2]$
  - Heat of pyrolysis: $L \in [4.2\ 10^5, 10^6]$ J/kg ... in non-conservative modellings !
- Convective heat transfer coefficient
  - $h \in [3.5, 34]$ W/m^2/K
  - Depends on the flow turbulence struture at the interface: constant value in any conditions ?
- **The (model-dependent) constants must be determined !**

Optimzed constants for PMMA

- *A priori* choice for several parameters
  - $c_{p,S,j} \approx 1100$ J/kg/K
  - $h \approx 10$ W/m^2/K in non-flaming conditions
  - A_S and E_a in the validity band experimentally observed for PMMA (Bal and Rein, 2013):

$$E_a = a \ln(As) + b, \quad a = 4.87\ 10^3,\ b \in [0, 5\ 10^4]$$

- Optimisation process (algorithm of Nelder and Mead, 1965) for the remaining parameters

$$\boldsymbol{p} = (A_{s,i}, b_i, n_i, L_i, c_{p,S,j}, \lambda_{S,j}, \kappa_{S,j}, \varepsilon_{S,j})$$

  applied simultaneously to both $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2 experiments.
- At least 7 relevant data sets $\mathcal{C}_1 - \mathcal{C}_7$ have been obtained.
  - $\mathcal{C}_1 - \mathcal{C}_3$: no internal radiation; $\mathcal{C}_4 - \mathcal{C}_7$: P1-radiation model
  - $\mathcal{C}_1 - \mathcal{C}_6$: constant $c_{p,S,j}$; $\mathcal{C}_7$: experimental $c_{p,S,j}$ (Agari et al., 1997)
- Discrepancies to the experimental results:
  - $\varphi_{\text{imp}} = 17$ kW/m^2: $< 5\%$ on the interface temperature, about 10% on the mass loss rate;
  - $\varphi_{\text{imp}} = 40$ kW/m^2: $< 1\%$ on the interface temperature, $< 5\%$ on the mass loss rate.

Results: comparison to the experiments of Kashiwagi and Ohlemiller, 1982

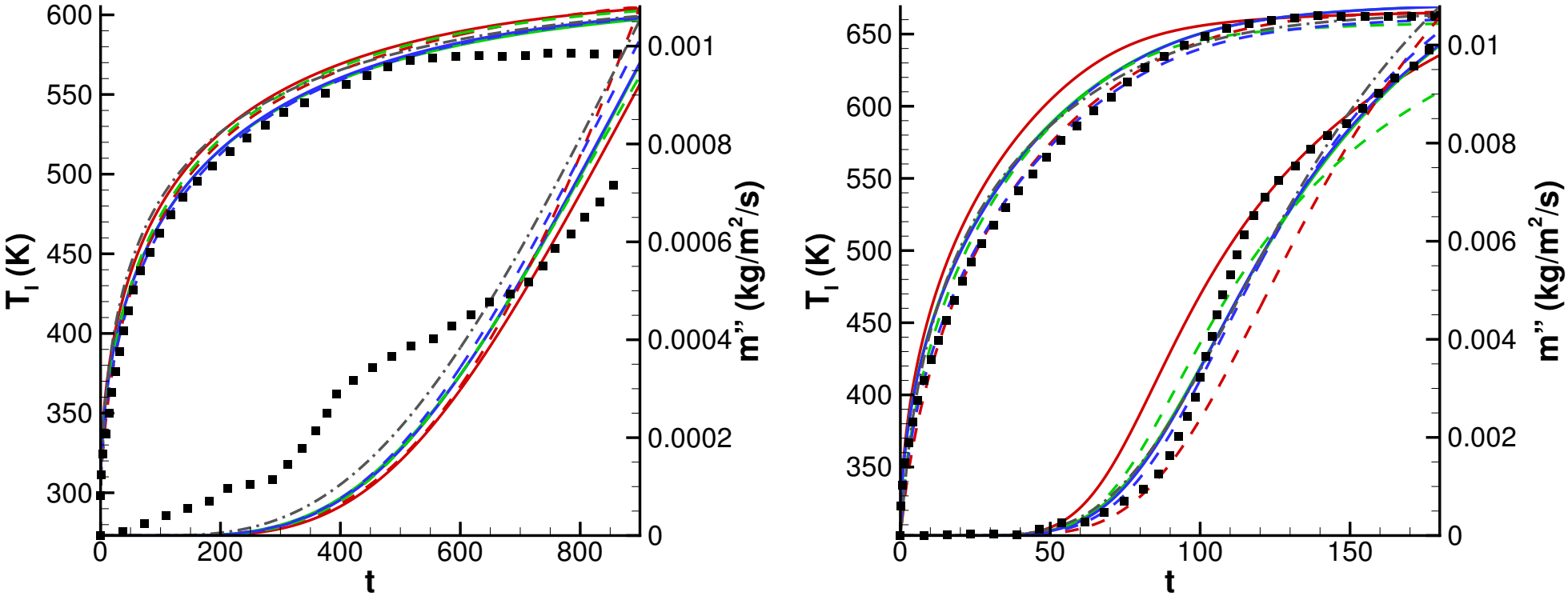


Figure : Comparison between the reference experimental results of Kashiwagi and Ohlemiller, 1982 (■) and the computed interface temperature (T) and mass loss rate ($\dot{m}''$)

Results: comparison to the experiments of Kashiwagi and Ohlemiller, 1982

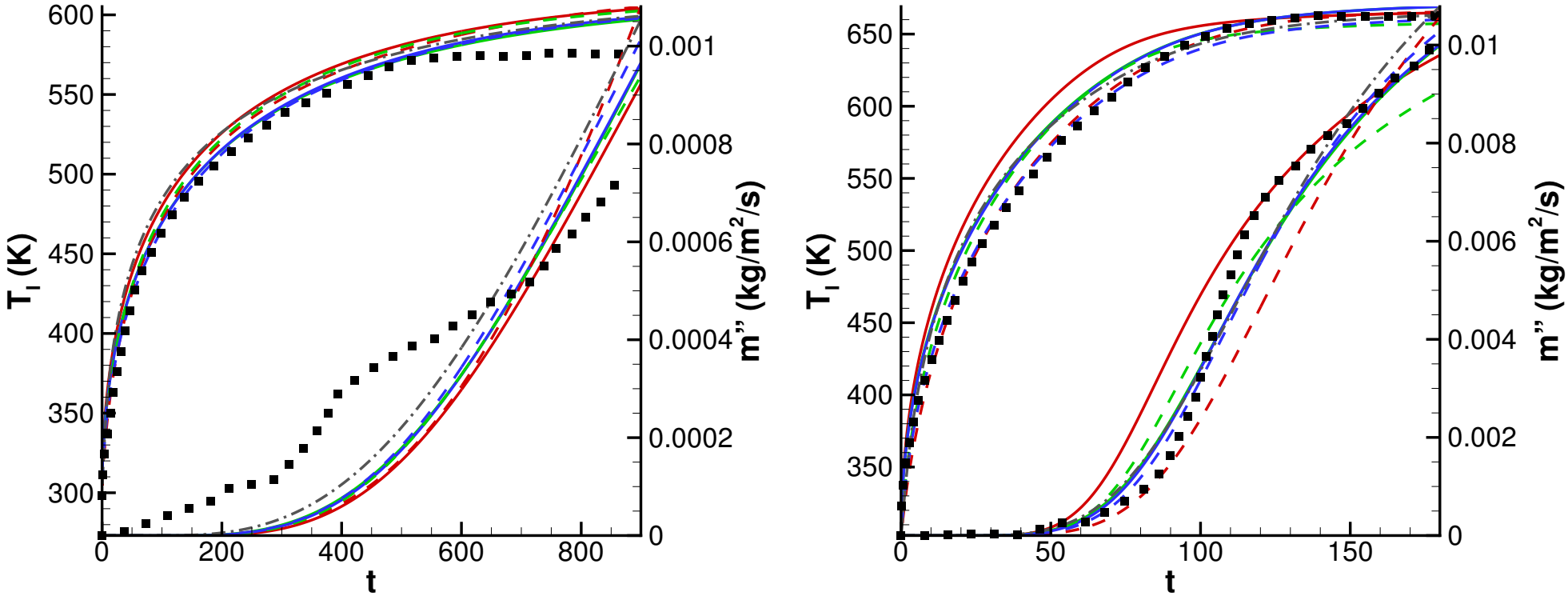


Figure : Comparison between the reference experimental results of Kashiwagi and Ohlemiller, 1982 (■) and the computed interface temperature (T) and mass loss rate ($\dot{m}''$)

- Numerical results in good agreement with the $\varphi_{\text{imp}} = 40$ kW/m^2-experiments
- At $\varphi_{\text{imp}} = 17$ kW/m^2:
  - steady state temperature not reached at $t = 900$ s contrary to the experiments
  - mass loss rate evolution not correctly reproduced
- Similar numerical results as Gpyro's (Lautenberger and Fernandez-Pello, 2009)

Outline

Limitations

- **Meaning of the current “validation”**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**

More selection criteria: i) Bubbled layer thickness

- Idea: the bubbled layer reaches a steady state thickness: $\delta \approx 3$ mm experimentally
- Possible definitions
  - $\rho_{\text{PMMA}}(\delta) = \rho_{\text{bPMMA}}(\delta)$
  - $\rho_{\text{bPMMA}}(\delta) = 0.99\rho^0_{\text{bPMMA}}$
  - ...

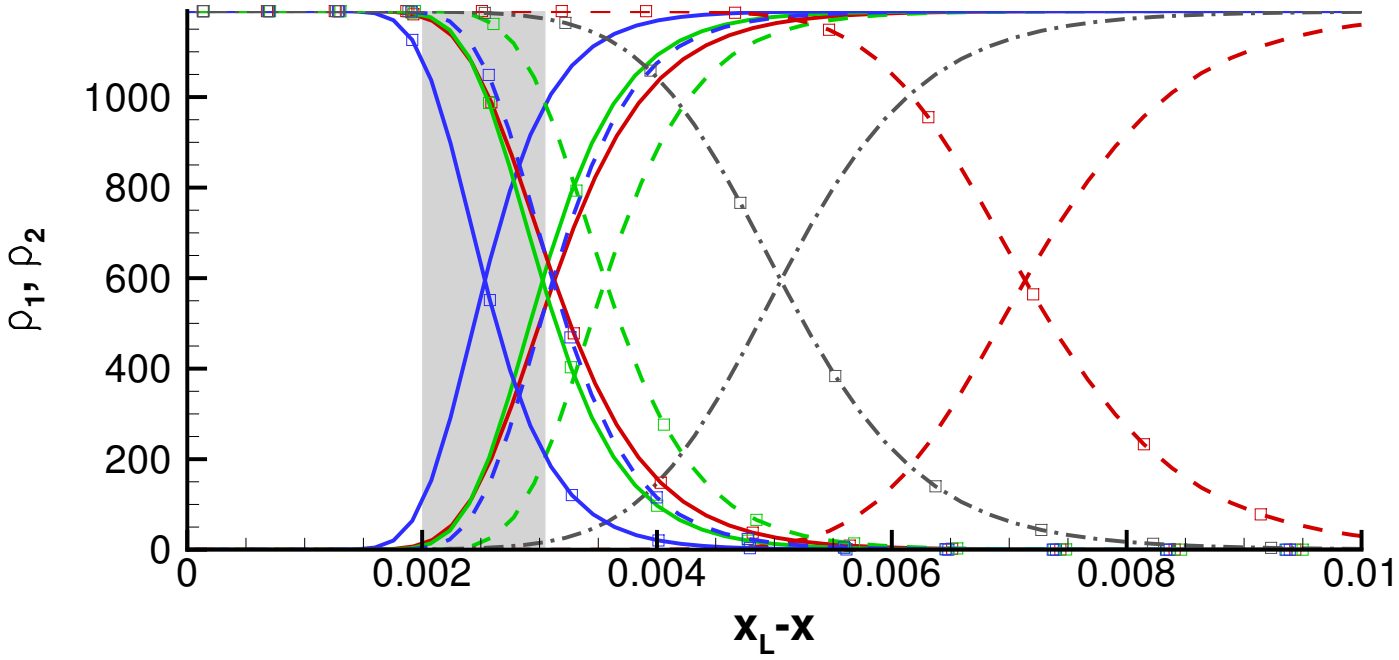


Figure : Partial densities profiles (ρ_{PMMA}: lines only; ρ_{bPMMA}: lines with squares) computed for an applied flux $\varphi_{\text{imp}} = 40$ kW/m^2 at $t = 180$ s. Shaded zone: observed bubbled zone thickness range.

- $\mathcal{C}_4$, $\mathcal{C}_7$ to be eliminated ?

More selection criteria: ii) Steady state mass loss rate

- Idea: PMMA pyrolysis approximately reaches a steady state behaviour with a temperature threshold and a constant mass loss rate
- The steady state mass loss rate evolves linearly with the total applied heat flux (experimental review of Lautenberger and Fernandez-Pello, 2009)
- For instance, $\dot{m}'' = 0.014$ kg/m^2/s at $\varphi_{\text{imp}} = 40$ kW/m^2 and $\dot{m}'' = 0.024$ kg/m^2/s at $\varphi_{\text{imp}} = 60$ kW/m^2

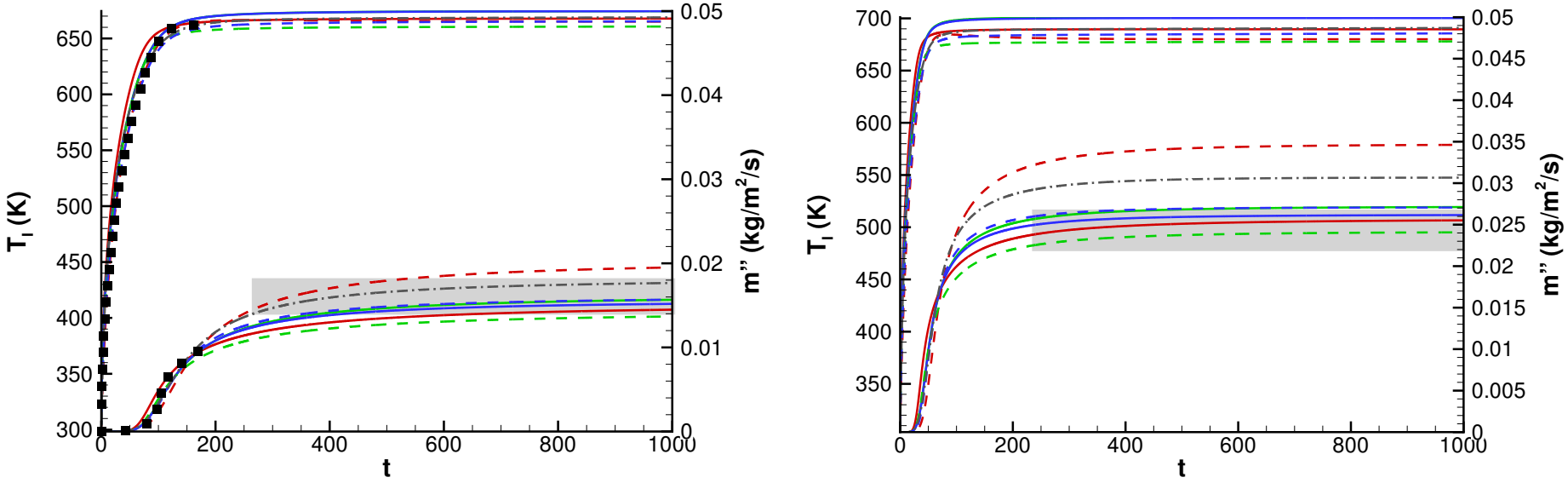


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2 (left) and $\varphi_{\text{imp}} = 60$ kW/m^2 (right). shaded zone: experimental steady mass loss rate values

- $\mathcal{C}_4$, $\mathcal{C}_7$ to be eliminated. . . again ?

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Case of the surface parameters h and ε: 40 % discrepancy on the mass loss rate

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Case of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of other modellings in CFD: radiation, turbulence, combustion

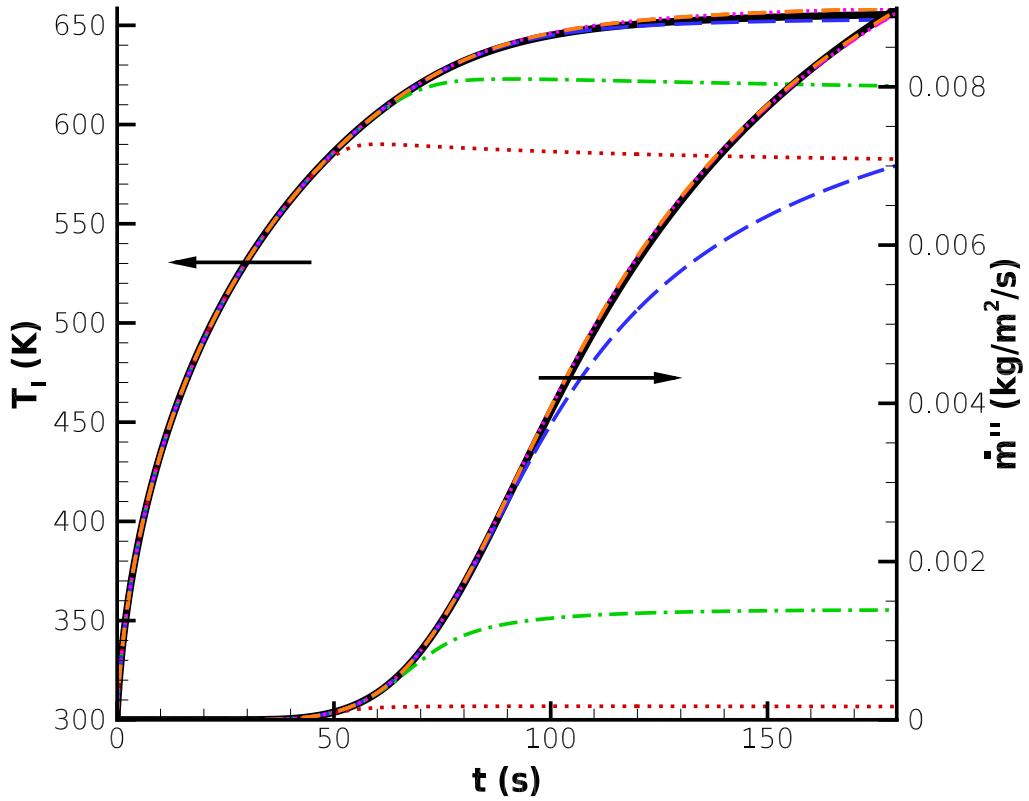
Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Case of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of other modellings in CFD: radiation, turbulence, combustion
- **Effect of missing phenomena in the current modelling ?**

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Case of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of other modellings in CFD: radiation, turbulence, combustion
- **Effect of missing phenomena in the current modelling ?**
  - **Example of the convective heat transfer in porous media**
  - Influence of the bubbled PMMA layer porosity ϕ

Comparison between monophasic and diphasic modellings



- Large dependance for $\phi_{S,2} \in [10^{-5}, 10^{-2}]$
- Convergence towards the monophasic results for $\phi_{S,2} > 10^{-2}$
- Assumed values of $\phi_{S,2}$:
  - $\phi_{S,2} \approx 0.1$ (Lautenberger and Fernandez-Pello, 2009)
  - $\phi_{S,2} \approx 0.001$ (Pizzo et al., 2015, visually)

Figure : Comparison between the monophasic (—) and the diphasic modellings ($\cdot$: $\phi_{S,2} = 10^{-5}$; $\cdot -$: $\phi_{S,2} = 10^{-4}$; $- - -$: $\phi_{S,2} = 10^{-3}$; $\cdot \cdot -$: $\phi_{S,2} = 10^{-2}$; $-$: $\phi_{S,2} = 10^{-1}$). Base data set: $\mathcal{C}_5$.

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Example of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of the surrounding physics in the fluid phase: radiation, turbulence, combustion
- **Effect of missing phenomena in the current modelling ?**
  - **Example of the convective heat transfer in porous media**
  - Influence of the bubbled PMMA layer porosity

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Example of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of the surrounding physics in the fluid phase: radiation, turbulence, combustion
- **Effect of missing phenomena in the current modelling ?**
  - **Example of the convective heat transfer in porous media**
  - Influence of the bubbled PMMA layer porosity
  - No account for O_2 concentration

Limitations

- **Meaning of the current "validation"**
  - Dependence of the parameter sets to possible remaining implementation errors...
  - ...and the modelling accuracy
- **Physical relevance of all the constant sets resulting from the optimization method ?**
- **The optimization process must include more physical criteria**. Examples:
  - **Existence of a bubbled layer in PMMA pyrolysis**
  - **Steady state mass loss rate ?**
  - Switch to flaming configurations ?
  - Switch to more complex computations (large scale PMMA flat plate)
- **Sensitivity to unknown parameters chosen in the "litterature range"**
  - Example of the surface parameters h and ε: 40 % discrepancy on the mass loss rate
  - Influence of the surrounding physics in the fluid phase: radiation, turbulence, combustion
- **Effect of missing phenomena in the current modelling ?**
  - **Example of the convective heat transfer in porous media**
  - Influence of the bubbled PMMA layer porosity
  - No account for O_2 concentration
  - Enhancement of the degradation path ?

Outline

Concluding remarks

- Questionable results obtained with a simple monophasic modelling used with optimized parameters
  - Not a proprer validation !
  - Fails to reproduce the initial pyrolysis behavior at lower incident flux
  - Parameter sets relevance to be evaluated at larger scale
  - Good agreement with large incident heat flux experiments
  - Provides good trends for long-term simulations

Concluding remarks

- Questionable results obtained with a simple monophasic modelling used with optimized parameters
  - Not a proprer validation !
  - Fails to reproduce the initial pyrolysis behavior at lower incident flux
  - Parameter sets relevance to be evaluated at larger scale
  - Good agreement with large incident heat flux experiments
  - Provides good trends for long-term simulations
- Need for a complementary analytical approach
  - A few reference materials to be completely characterized (heat transfers, thermochemistry, etc.)
  - Special care on the the thermal degradation process (reactive path independent from the imposed temperature raise)
  - Need for a complete modelling (radiative, convective heat transfers; temperature-dependent parameters; 3D pyrolysis; etc...)
  - Necessary approach to carry out a modelling validation and predictive simulations

Concluding remarks

- Questionable results obtained with a simple monophasic modelling used with optimized parameters
  - Not a proprer validation !
  - Fails to reproduce the initial pyrolysis behavior at lower incident flux
  - Parameter sets relevance to be evaluated at larger scale
  - Good agreement with large incident heat flux experiments
  - Provides good trends for long-term simulations
- Need for a complementary analytical approach
  - A few reference materials to be completely characterized (heat transfers, thermochemistry, etc.)
  - Special care on the the thermal degradation process (reactive path independent from the imposed temperature raise)
  - Need for a complete modelling (radiative, convective heat transfers; temperature-dependent parameters; 3D pyrolysis; etc...)
  - Necessary approach to carry out a modelling validation and predictive simulations
- Long-term additional modellings
  - 3D pyrolysis: vertical flat plate, porous media such as cable trays
  - Specific cable trays convective and radiative heat transfers models

Concluding remarks

- Questionable results obtained with a simple monophasic modelling used with optimized parameters
  - Not a proprer validation !
  - Fails to reproduce the initial pyrolysis behavior at lower incident flux
  - Parameter sets relevance to be evaluated at larger scale
  - Good agreement with large incident heat flux experiments
  - Provides good trends for long-term simulations
- Need for a complementary analytical approach
  - A few reference materials to be completely characterized (heat transfers, thermochemistry, etc.)
  - Special care on the the thermal degradation process (reactive path independent from the imposed temperature raise)
  - Need for a complete modelling (radiative, convective heat transfers; temperature-dependent parameters; 3D pyrolysis; etc...)
  - Necessary approach to carry out a modelling validation and predictive simulations
- Long-term additional modellings
  - 3D pyrolysis: vertical flat plate, porous media such as cable trays
  - Specific cable trays convective and radiative heat transfers models
- Need for a "modelling balance" between all the involved physical phenomena !

Thank you for your attention

Bibliography


Nelder, J. A. and R. Mead (1965). "A Simplex Method for Function Minimization". In: *The Computer Journal* 7.4, pp. 308–313. DOI: 10.1093/comjnl/7.4.308.


Kashiwagi, Takashi and Thomas J. Ohlemiller (1982). "A study of oxygen effects on nonflaming transient gasification of PMMA and PE during thermal irradiation". In: *Symposium (International) on Combustion* 19.1. Nineteenth Symposium (International) on Combustion, pp. 815 –823. DOI: http://dx.doi.org/10.1016/S0082-0784(82)80257-9.


Kuo, Kenneth K. (1986). *Principles of Combustion*. John Wiley & Sons, Inc.


Agari, Y. et al. (1997). "Thermal diffusivity and conductivity of PMMA/PC blends". In: *Polymer* 38.4, pp. 801 –807. DOI: http://dx.doi.org/10.1016/S0032-3861(96)00577-0.


Lautenberger, C. W. and A. C. Fernandez-Pello (2009). "Generalized pyrolysis model for combustible solids". In: *Fire Safety Journal* 44, pp. 819–839.


Bal, N. and G. Rein (2013). "Relevant model complexity for non-charring polymer pyrolysis". In: *Fire Safety Journal* 61, pp. 36–44.


Ghorbani, Zohreh et al. (2013). "Limitations in the predictive capability of pyrolysis models based on a calibrated semi-empirical approach". In: *Fire Safety Journal* 61.0, pp. 274 –288.


Pizzo, Yannick et al. (2015). "Steady and transient pyrolysis of thick clear PMMA slabs". In: *Combustion and Flame* 162.1, pp. 226–236. DOI: http://dx.doi.org/10.1016/j.combustflame.2014.07.004.

Outline

Multi-species pyrolysis

- Solid phase
  - $S_1, \ldots, S_{N_S}$: solid species
  - Phasic densities $\rho^0_{S,j}(T_S)$: species mass over species volume
  - Partial densities $\rho_{S,j}$: species mass over total solid volume
  - Deformation velocity $\mathbf{u}_{e,S}$
- Gas phase
  - $G_1, \ldots, G_{N_G}$: gaseous species
  - Instantaneous ejection from the solid domain
  - Interface mass flow rate: partial densities $\rho_{G,j}$, mass fractions $Y_{G,j} = \rho_{G,j}/\rho_G$
  - Species velocity $\mathbf{u}_{e,G,j}$, average gaseous velocity $\rho_G \mathbf{u}_{e,G} = \sum_{j=1}^{N_G} \rho_{G,j} \mathbf{u}_{e,G,j}$
- Degradation reactions
  - $\mathcal{R}_1, \ldots, \mathcal{R}_{N_R}$ such as

(1) $$\mathcal{R}_i \ : \quad \sum_{j=1}^{N_S} \mu'_{ij} S_j \ + \sum_{j=1}^{N_G} \nu'_{ij} G_j \ \longrightarrow \ \sum_{j=1}^{N_S} \mu''_{ij} S_j \ + \sum_{j=1}^{N_G} \nu''_{ij} G_j$$

  - Mass stoechiometric coefficients $\mu'_i, \mu''_{ij}, \nu'_{ij}, \nu''_{ij}$ such as

(2) $$\sum_{j=1}^{N_S} (\mu'_{ij} - \mu''_{ij}) + \sum_{j=1}^{N_G} (\nu'_{ij} - \nu''_{ij}) = 0 \quad \text{and} \quad \sum_{j=1}^{N_S} \mu_{ij} < 0 \quad \forall \ i$$

  - Reaction rates modelled by Arrhenius laws:

(3) $$\dot{\omega}_i = \rho_{S,0} A_{S,i} e^{\frac{-E_{a,i}}{RT_S}} \left(\frac{\rho_{S,i}}{\rho_{S,0}} \right)^{\alpha_i}$$

Conservation equations: mass and volume

- Solid species

$$\partial_t \rho_{S,j} + \boldsymbol{\nabla} \cdot \left(\rho_{S,j} \mathbf{u}_{e,S}\right) = \sum_{i=1}^{N_R} \mu_{ij} \dot{\omega}_i \tag{4}$$

- Solid volume

$$\boldsymbol{\nabla} \cdot \mathbf{u}_{e,S} = \sum_{j=1}^{N_S} \rho_{S,j} \left(\partial_t (1/\rho^0_{S,j}) + \mathbf{u}_{e,S} \cdot \boldsymbol{\nabla}(1/\rho^0_{S,j})\right) + \sum_{i=1}^{N_R} \frac{\mu_{ij} \dot{\omega}_i}{\rho^0_{S,j}} \tag{5}$$

- Solid mass loss ($\sum_{i=1}^{N_R} (4)_j$)

$$\partial_t \rho_S + \boldsymbol{\nabla} \cdot \left(\rho_S \mathbf{u}_{e,S}\right) = \sum_{i=1}^{N_R} \left[\sum_{j=1}^{N_S} \mu_{ij}\right] \dot{\omega}_i \tag{6}$$

- Mass flux at the fluid/solid interface (instantaneous ejection):

$$\begin{aligned} \int_{\Gamma_{\text{out}}} \rho_{G,j} \left(\mathbf{u}_{e,G,j} - \mathbf{u}_{e,S}\right) \cdot \mathbf{n} \, \mathrm{d}\sigma &= \int_{\Omega_S^{\text{tot}}} \left[\sum_{i=1}^{N_R} \nu_{ij} \dot{\omega}_i\right] \mathrm{d}\mathcal{V} \\ \dot{m}'' = \int_{\Gamma_{\text{out}}} \rho_G \left(\mathbf{u}_{e,G} - \mathbf{u}_{e,S}\right) \cdot \mathbf{n} \, \mathrm{d}\sigma &= \int_{\Omega_S^{\text{tot}}} \sum_{i=1}^{N_R} \left[\sum_{j=1}^{N_S} \nu_{ij} \dot{\omega}_i\right] \mathrm{d}\mathcal{V} \end{aligned} \tag{7}$$

Conservation equations: enthalpy

- Fundamental hypothesis: enthalpy (h) conservation of the whole system { gas + solid }
- Enthalpy decomposition: formation Δh_f^0 plus sensible $\tilde{h}$
- Conservative expression on the solid domain

$$\partial_t(\rho_S \tilde{h}_S) + \boldsymbol{\nabla} \cdot (\rho_S \tilde{h}_S \mathbf{u}_{e,S}) = -\sum_{i=1}^{N_R} L_i \dot{\omega}_i + \boldsymbol{\nabla} \cdot (\lambda \boldsymbol{\nabla} T) - \boldsymbol{\nabla} \cdot \boldsymbol{q}_{\text{rad}} \tag{8}$$

Heat of pyrolysis associated to each degradation reaction:

$$L_i = \left(\sum_{j=1}^{N_S} \mu_{ij} \Delta h^0_{S,f,j} + \sum_{j=1}^{N_G} \nu_{ij} \Delta h^0_{g,f,j} \right)$$

- P1 internal radiation model
  - Radiative heat flux vector defined as $\boldsymbol{q}_{\text{rad}} = -\boldsymbol{\nabla} G / 3\kappa$
  - G: spheric integral of the radiation intensity
  - κ: radiative absorption coefficient)
  - Incident radiation transport equation:

$$-\boldsymbol{\nabla} \cdot (\boldsymbol{q}_{\text{rad}}) = \boldsymbol{\nabla} \cdot \left(\frac{1}{3\kappa} \boldsymbol{\nabla} G \right) = \kappa G - 4\kappa\sigma_B T^4 \tag{9}$$

Conservation equations: thermal fluid-solid interaction at the interface

- Boundary condition at the fluid/solid interface

$$\boldsymbol{q}_{\text{rad}} \cdot \mathbf{n} = \varepsilon_S \varphi_{\text{imp}}$$

$$\lambda \boldsymbol{\nabla} T \cdot \mathbf{n} + h(T_I - T_F) + \varepsilon_S \sigma_B (T_I^4 - T_F^4) + \sum_{j=1}^{N_G} \rho_{G,j} \tilde{h}_{G,j} (\mathbf{u}_{e,G,j} - \mathbf{u}_{e,S}) \cdot \mathbf{n} = 0$$

with

  - T_I: interface temperature; $T_F = \lim_{x \to x_I} T(x)$;
  - $\varphi_{\text{rad,abs}} = \varepsilon_S \varphi_{\text{imp}}$ radiative flux transmitted into the solid;
  - $\varphi_{\text{rad,e}} = \varepsilon_S \sigma (T_I^4 - T_F^4)$ radiatif flux emitted by the solid surface;
  - φ_{imp} overall imposed radiative heat flux
  - $\mathbf{n}$ solid outward unit normal vector.

- Case of an opaque solid
  - No radiative heat transfer equation, $\boldsymbol{q}_{\text{rad}}$ in the solid domain
  - Modified boundary condition which includes the surfacic radiative heat transfer

$$\lambda \boldsymbol{\nabla} T \cdot \mathbf{n} + h(T_I - T_F) + \varepsilon_S \sigma_B (T_I^4 - T_F^4) - \varepsilon_S \varphi_{\text{imp}} + \sum_{j=1}^{N_G} \rho_{G,j} \tilde{h}_{G,j} (\mathbf{u}_{e,G,j} - \mathbf{u}_{e,S}) \cdot \mathbf{n} = 0$$

Account for the porosity effects (1)

- Basic assumption: multiphase termal equilibrium, $T_G = T_S = T$
- Porosity
  - Total porosity:

$$\phi \;=\; \delta\mathcal{V}_G/\delta\mathcal{V} \;=\; \sum_{j=1}^{N_S} \frac{\rho_{S,j}}{\rho^0_{S,j}}$$

    where $\rho_{S,j}$ are the solid species partial densities and $\rho^0_{S,j}$ their intrinisic phase densities.
  - Solid species partial porosity $\phi_{S,j}$ such that

$$\phi \;=\; \sum_{j=1}^{N_S} \frac{\rho_{S,j}\phi_{S,j}}{\rho^0_{S,j}(1-\phi_{S,j})} \quad \text{and} \sum_{j=1}^{N_S} \frac{\rho_{S,j}}{\rho^0_{S,j}(1-\phi_{S,j})} \;=\; 1$$

- Gas phase notations
  - Gas phase density ρ_G, dynamic pressure p_G, thermodynamic pressure P_{th};
  - Mass fractions $Y_{G,j}$ an molar masses $W_{G,j}$ such that

$$\frac{1}{W_G} \;=\; \sum_{j=1}^{N_G} \frac{Y_{G,j}}{W_{G,j}} \quad \text{and} \quad \sum_{j=1}^{N_G} Y_{G,j} \;=\; 1$$

  - Relation between density, thermdynamic pressure and average molar mass W_G:

$$\rho_G \;=\; \frac{P_{\text{th}}\, W_G}{RT}$$

Account for the porosity effects (2)

- Gaseous species conservation

$$\partial_t(\rho_G \phi Y_{G,j}) + \boldsymbol{\nabla} \cdot (\rho_G \phi Y_{G,j} \mathbf{u}_{e,G}) - \boldsymbol{\nabla} \cdot (D \boldsymbol{\nabla} Y_{G,j}) = \sum_{i=1}^{N_R} \sum_{j=1}^{N_G} \nu_{ij} \dot{\omega}_i$$

- Gas density conservation:

$$\partial_t(\rho_G \phi) + \boldsymbol{\nabla} \cdot (\rho_G \phi \mathbf{u}_{e,G}) = \sum_{i=1}^{N_R} \sum_{j=1}^{N_G} \nu_{ij} \dot{\omega}_i$$

- Pressure-gradient driven gas velocity: Darcy law

$$\mathbf{u}_{e,G} = -\frac{K}{\mu} \boldsymbol{\nabla} p_G$$

- The combination of the Darcy law with the gas density conservation equation allows to solve a linear elliptic equation for p_G
- Boundary conditions
  - $p_G = 0$ at $x = x_L$; $\partial_n p_G = 0$ at $x = 0$ (zero-velocity)
  - $\partial_n Y_{G,j} = 0$ on both sides.

Numerical method: principles

- Implementation of a demonstration software for 1D pyrolysis
- Arbitrary Lagrangian-Eulerian discretization
  - $\mathbf{u}_a$: mesh deformation velocity which coincides with the overall solid deformation
  - Transformation of the conservation equations (example of a quantity f):

$$\frac{\mathrm{d}}{\mathrm{d}t}\left[\int_K f \,\mathrm{d}\mathcal{V}\right] + \int_{\partial K} f_\sigma (\mathbf{u} - \mathbf{u}_a)_\sigma \cdot \mathbf{n} \,\mathrm{d}\sigma = \int_K q \,\mathrm{d}\mathcal{V}$$

- First-order backward-Euler time discretization
- Finite volume discretization
  - centered schemes for the convective terms
  - centered diffusion
- Stability
  - Enthalpy: ensured by the diffusive term and the wellposedness of the continuous conservation law
  - Mass: ensured by the degradation laws ($\sum_{j=1}^{N_S} \mu_{ij} < 0 \quad \forall\ i$)

Outline

Constants optimisation method

- Demonstration pyrolysis code coupled with an optimisation method
  - Nelder & Mead simplex method (Nelder and Mead, 1965)
  - cost function relative to the input parameters $\boldsymbol{p}$ and an experimental case c to minimize

$$f_c(\boldsymbol{p}) = \alpha_T \frac{\| T_{I,\text{num}}(\boldsymbol{p}) - T_{I,\text{exp}} \|_t^2}{\| T_{I,\text{num}}(\boldsymbol{p}) \|_t^2} + \alpha_m \frac{\| \dot{m}''_{\text{num}}(\boldsymbol{p}) - \dot{m}_{\text{exp}} \|^2}{\| \dot{m}''_{\text{num}}(\boldsymbol{p}) \|^2}, \quad \alpha_T + \alpha_m = 1$$

  - overall cost function relative to both $\varphi_{\text{imp}} = 17$ kW/m^2 and $\varphi_{\text{imp}} = 40$ kW/m^2 experiments:

$$f(\boldsymbol{p}) = f_{17\text{kW/m}^2}(\boldsymbol{p}) + f_{40\text{kW/m}^2}(\boldsymbol{p})$$

- Some hints on the parameters
  - $c_{p,S,j} \approx 1100$ J/kg/K
  - $h \approx 10$ W/m^2/K in non-flaming conditions
  - Relation between A_S and E_a for PMMA (Bal and Rein, 2013):

$$E_a = a \ln(As) + b, \quad a = 4.87\,10^3, \; b \in [0, 5\,10^4]$$

- Conclusion: parameters to determine:

$$\boldsymbol{p} = (A_{s,i}, b_i, n_i, L_i, c_{p,S,j}, \lambda_{S,j}, \kappa_{S,j}, \varepsilon_{S,j})$$

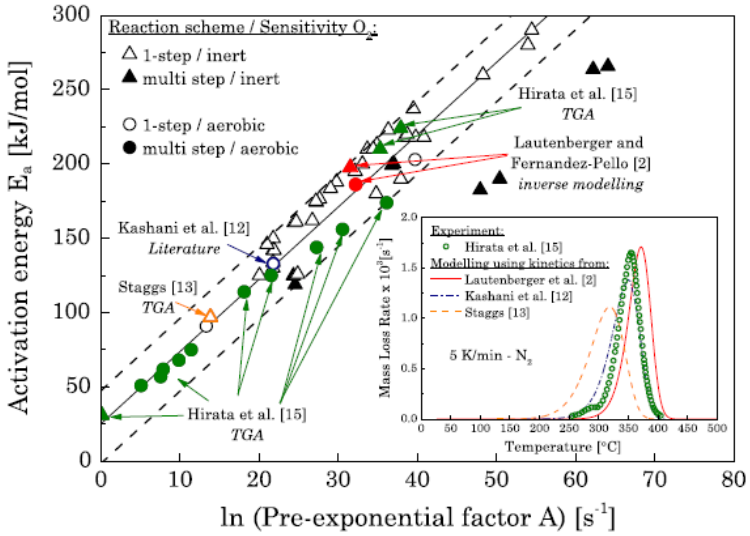


Figure : PMMA admissible zone for $(\ln(A_S), E_a)$ (Bal and Rein, 2013)

Results: comparison to the experiments of Kashiwagi and Ohlemiller, 1982

	Opaque			P1 radiation model			
	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$
$A_{S,1}$ (s^{-1})	$1.0\ 10^{10}$	$1.52\ 10^{10}$	$2.75\ 10^{10}$	$1.34\ 10^{8}$	$1.13\ 10^{10}$	$1.45\ 10^{9}$	$1.96\ 10^{8}$
$A_{S,2}$ (s^{-1})	$1.0\ 10^{13}$	$1.73\ 10^{10}$	$4.18\ 10^{10}$	$4.44\ 10^{9}$	$5.51\ 10^{11}$	$2.28\ 10^{10}$	$2.72\ 10^{10}$
$E_{a,i}$ (kJ/mol)	(116, 184)	(114, 150)	(117, 155)	(91.1, 165)	(115, 161)	(102, 154)	(94.2, 167)
$n_{R,i}$	(1.0, 1.04)	(1.0, 1.0)	(1.0, 1.0)	(1.25, 1.98)	(1.0, 1.0)	(1.0, 1.0)	(1.43, 1.42)
L_2 (J/kg)	$1.12\ 10^{6}$	$1.01\ 10^{6}$	$1.24\ 10^{6}$	$7.20\ 10^{5}$	$1.47\ 10^{6}$	$1.32\ 10^{6}$	$7.72\ 10^{5}$
$\rho^0_{S,j}$ (kg/m^3)	1190	1190	1190	1190	1190	1190	1190
$c_{p,S,j}$ (J/kg/K)	2100	2500	3000	1600	2500	3000	Exp.
$\lambda_{p,S,j}$ (W/m/K)	0.2	0.2	0.2	0.2	0.2	0.2	Exp.
$\kappa_{p,S,j}$ (m^{-1})	N/A	N/A	N/A	1000	3270	4000	Lin.
h ($W/m^2/K$)	10	10	10	10	10	10	10
ε_j	0.86	0.85	0.85	0.86	0.95	0.96	0.85
$c_{p,G}$ (J/kg/K)	1100	1100	1100	1100	1100	1100	1100

Table : Set of constants obtained by optimisation with respect to Kashiwagi and Ohlemiller, 1982 experiments. Exp.: constants imposed to the values determined by Agari et al., 1997; Lin.: $\kappa(T) = \kappa_0 + \kappa_1(T - T_0), \kappa_0 = 1000\ m^{-1}$, $\kappa_1 = 10\ m^{-1}/K$, $T_0 = 300\ K$.

Results: comparison to the experiments of Kashiwagi and Ohlemiller, 1982

	Opaque			P1 radiation model			
	$\mathcal{C}_1$	$\mathcal{C}_2$	$\mathcal{C}_3$	$\mathcal{C}_4$	$\mathcal{C}_5$	$\mathcal{C}_6$	$\mathcal{C}_7$
$A_{S,1}$ (s^{-1})	$1.0\ 10^{10}$	$1.52\ 10^{10}$	$2.75\ 10^{10}$	$1.34\ 10^{8}$	$1.13\ 10^{10}$	$1.45\ 10^{9}$	$1.96\ 10^{8}$
$A_{S,2}$ (s^{-1})	$1.0\ 10^{13}$	$1.73\ 10^{10}$	$4.18\ 10^{10}$	$4.44\ 10^{9}$	$5.51\ 10^{11}$	$2.28\ 10^{10}$	$2.72\ 10^{10}$
$E_{a,i}$ (kJ/mol)	(116, 184)	(114, 150)	(117, 155)	(91.1, 165)	(115, 161)	(102, 154)	(94.2, 167)
$n_{R,i}$	(1.0, 1.04)	(1.0, 1.0)	(1.0, 1.0)	(1.25, 1.98)	(1.0, 1.0)	(1.0, 1.0)	(1.43, 1.42)
L_2 (J/kg)	$1.12\ 10^{6}$	$1.01\ 10^{6}$	$1.24\ 10^{6}$	$7.20\ 10^{5}$	$1.47\ 10^{6}$	$1.32\ 10^{6}$	$7.72\ 10^{5}$
$\rho^0_{S,j}$ (kg/m^3)	1190	1190	1190	1190	1190	1190	1190
$c_{p,S,j}$ (J/kg/K)	2100	2500	3000	1600	2500	3000	Exp.
$\lambda_{p,S,j}$ (W/m/K)	0.2	0.2	0.2	0.2	0.2	0.2	Exp.
$\kappa_{p,S,j}$ (m^{-1})	N/A	N/A	N/A	1000	3270	4000	Lin.
h ($W/m^2/K$)	10	10	10	10	10	10	10
ε_j	0.86	0.85	0.85	0.86	0.95	0.96	0.85
$c_{p,G}$ (J/kg/K)	1100	1100	1100	1100	1100	1100	1100

Table : Set of constants obtained by optimisation with respect to Kashiwagi and Ohlemiller, 1982 experiments. Exp.: constants imposed to the values determined by Agari et al., 1997; Lin.: $\kappa(T) = \kappa_0 + \kappa_1(T - T_0), \kappa_0 = 1000\ m^{-1}$, $\kappa_1 = 10\ m^{-1}/K$, $T_0 = 300\ K$.

- Gap between the computed and experimental results
  - $\varphi_{imp} = 17\ kW/m^2$: $< 5\%$ on the interface temperature, about 10% on the mass loss rate;
  - $\varphi_{imp} = 40\ kW/m^2$: $< 1\%$ on the interface temperature, $< 5\%$ on the mass loss rate.

Material variability and modelling deficiencies

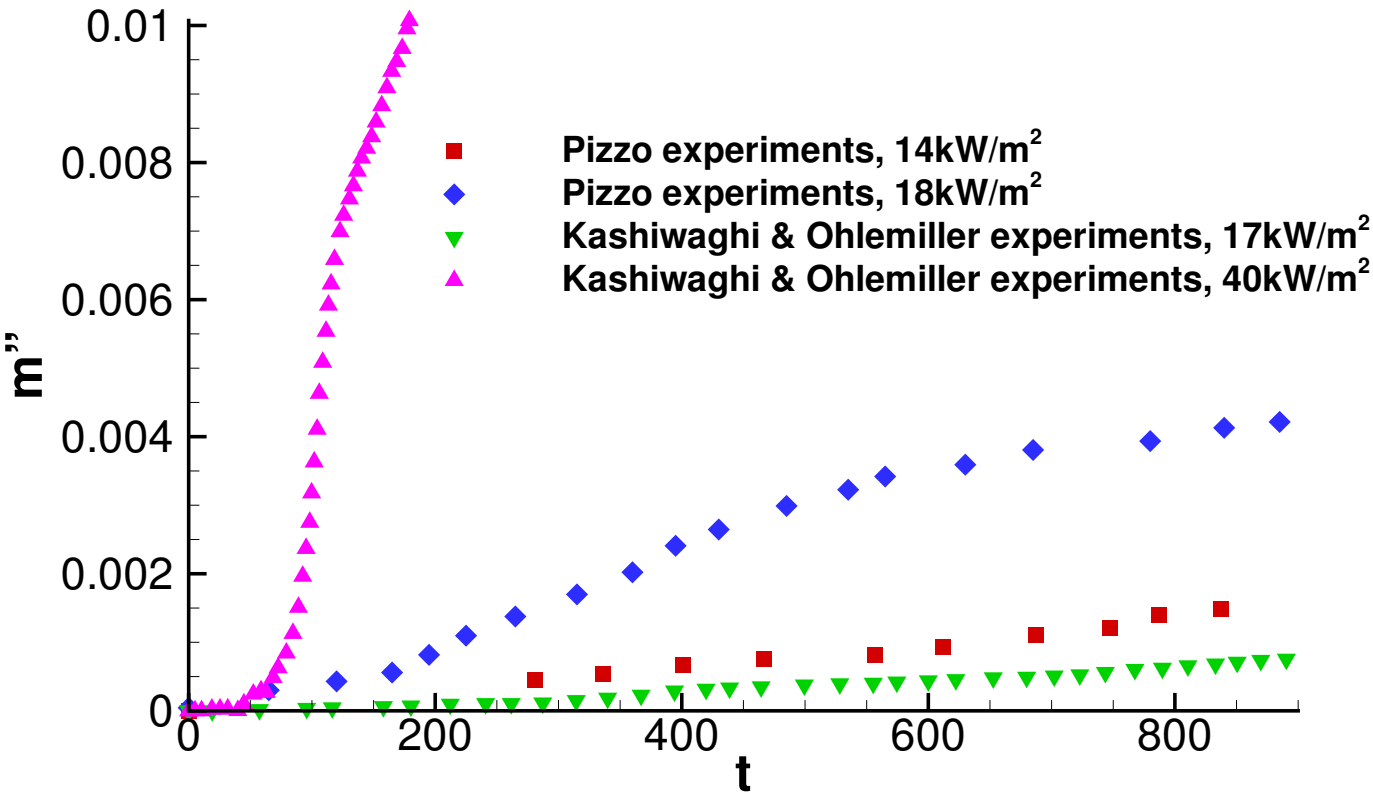


Figure : Mass loss rate evolution. Comparison between Kashiwaghi & Ohlemiller and Pizzo Pizzo et al., 2015 experiments under 20% O_2

Material variability and modelling deficiencies

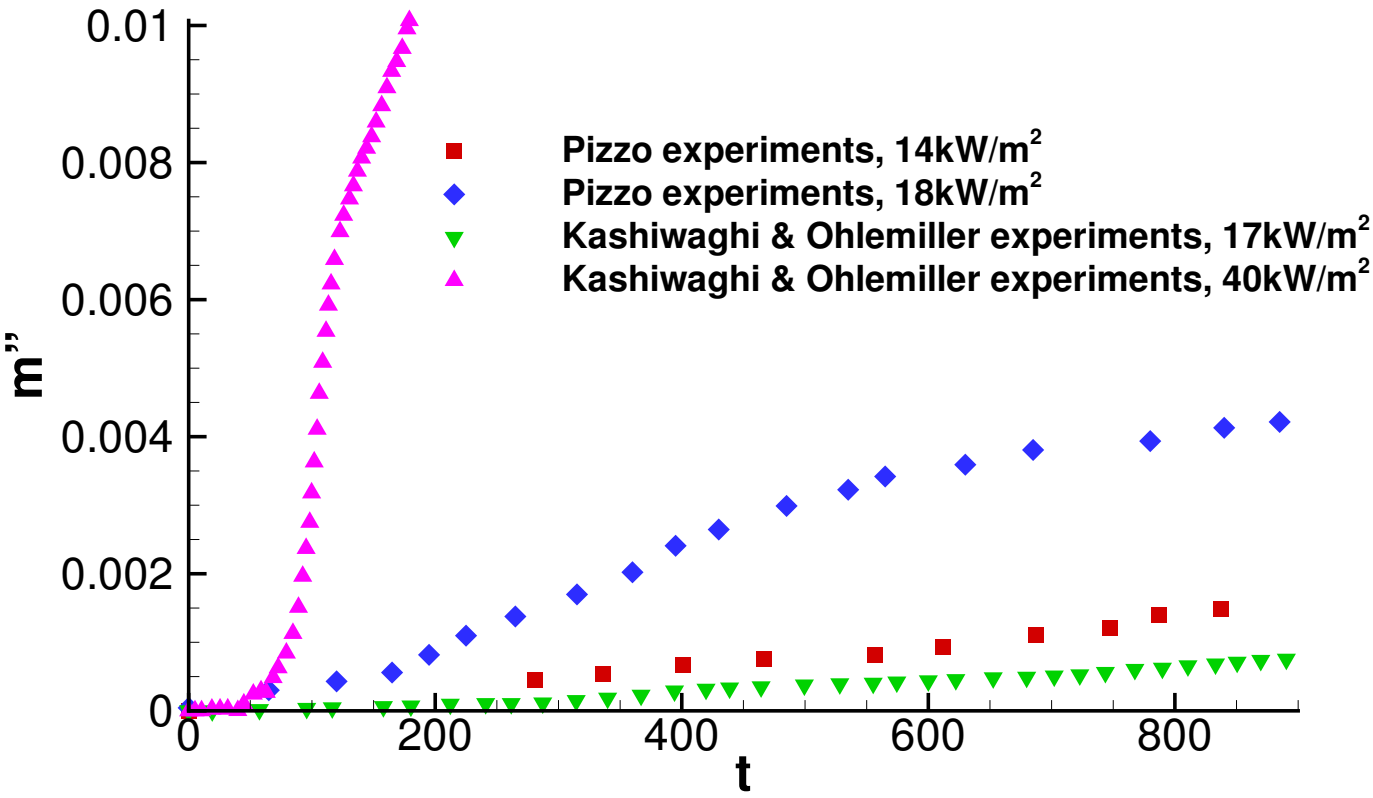


Figure : Mass loss rate evolution. Comparison between Kashiwaghi & Ohlemiller and Pizzo Pizzo et al., 2015 experiments under 20% O_2

- One could expect $\dot{m}''_{17\ \mathrm{kW/m^2}}$ closer from $\dot{m}''_{18\ \mathrm{kW/m^2}}$ than from $\dot{m}''_{14\ \mathrm{kW/m^2}}$
- **Differencies in the tested PMMA properties ?**

Material variability and modelling deficiencies

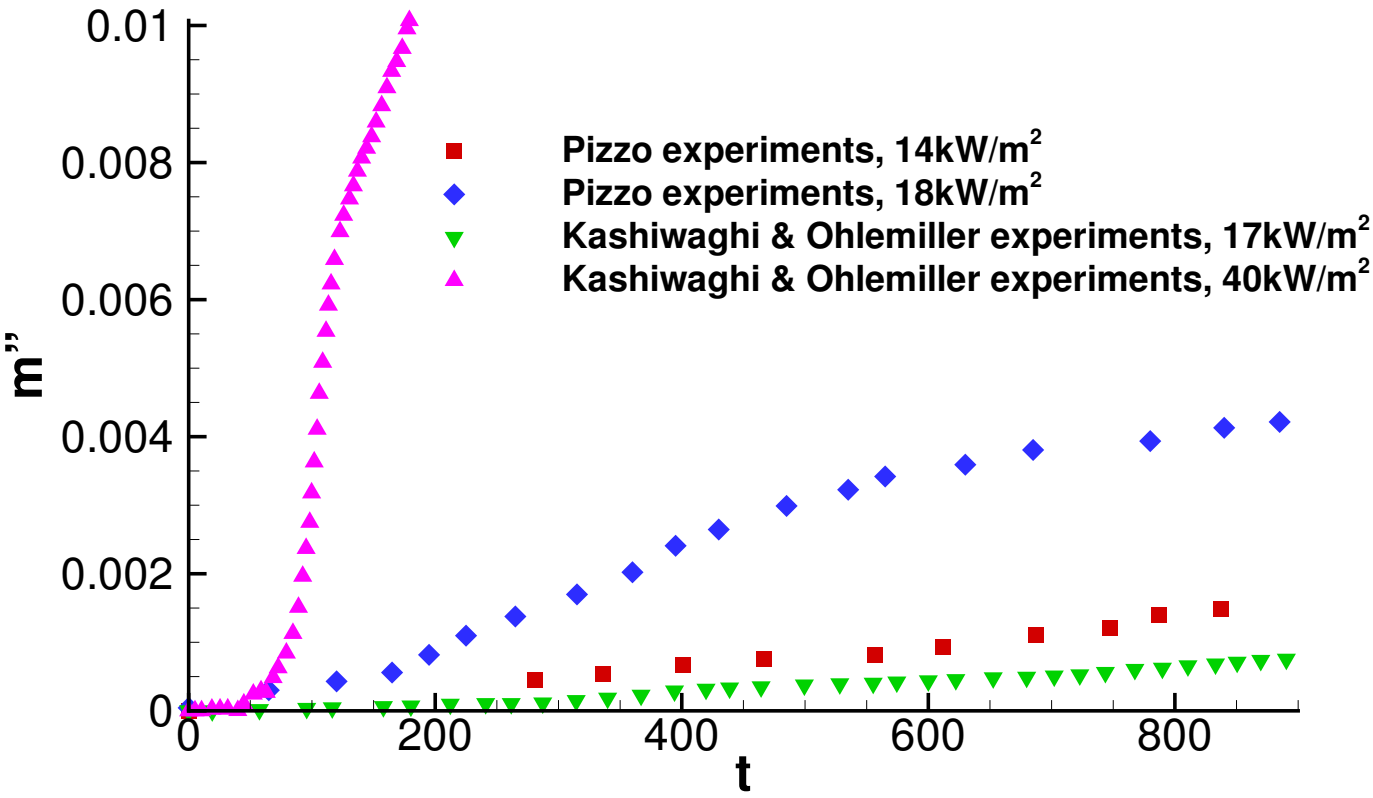


Figure : Mass loss rate evolution. Comparison between Kashiwaghi & Ohlemiller and Pizzo Pizzo et al., 2015 experiments under 20% O_2

- One could expect $\dot{m}''_{17\ \mathrm{kW/m^2}}$ closer from $\dot{m}''_{18\ \mathrm{kW/m^2}}$ than from $\dot{m}''_{14\ \mathrm{kW/m^2}}$
- **Differencies in the tested PMMA properties ?**
- A new optimization process may be necessary
- **Generic consideration of the O_2 concentration ?**

Comparison to Pizzo experiments

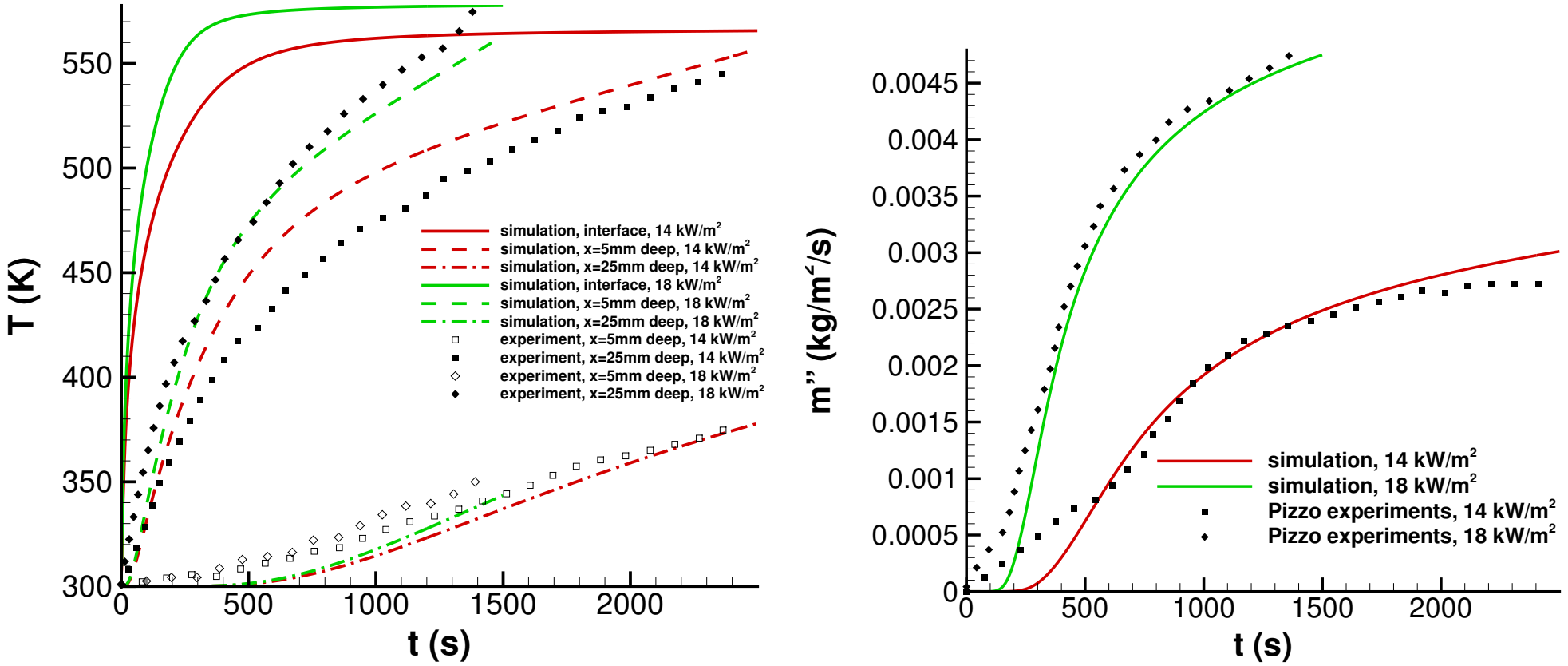


Figure : Comparison between the experimental results of Pizzo and the related simulations. Left: temperature; right: mass loss rate.

- Remark: available temperature at $x = 5$ mm and $x = 25$ mm from the interface
- Same quantitative error between the computed and experimental temperatures as in Kashiwagi & Ohlemiller case
- Even better agreement on the mass loss rates, except in the early stages of the experiment (initial linear growth)

Outline

Sensitivity to ill-known parameters

- The thermophysic parameters may be characterized with reasonable reliability in DSC
- No *a priori* knowledge about the thermokinetic constants (A_s, E_a, n_R, L)
- Interface heat transfer parameters:
  - wide range for the surface emissivity in litterature
  - difficult evaluation of the convective heat transfers (turbulence models. . .)
- Additional difficulty of the radiative heat transfers in the solid
- Base parameters for the sensitivity study
  - $A_s = (10^{10}, 10^{13})$ s^{-1}, $E_a = (1.16\ 10^5 1.91\ 10^5)$ kJ/mol, $N_R = 1$;
  - $L_2 = 2\ 10^6$ J/kg, $c_{p,G} = 1100$ J/kg/K
  - $c_{p,S}, \lambda_S$: experimental characterizations κ_S: linear growth
  - $h = 10$ W/m/K, $\varepsilon = 0.9$

Sensitivity to A_s

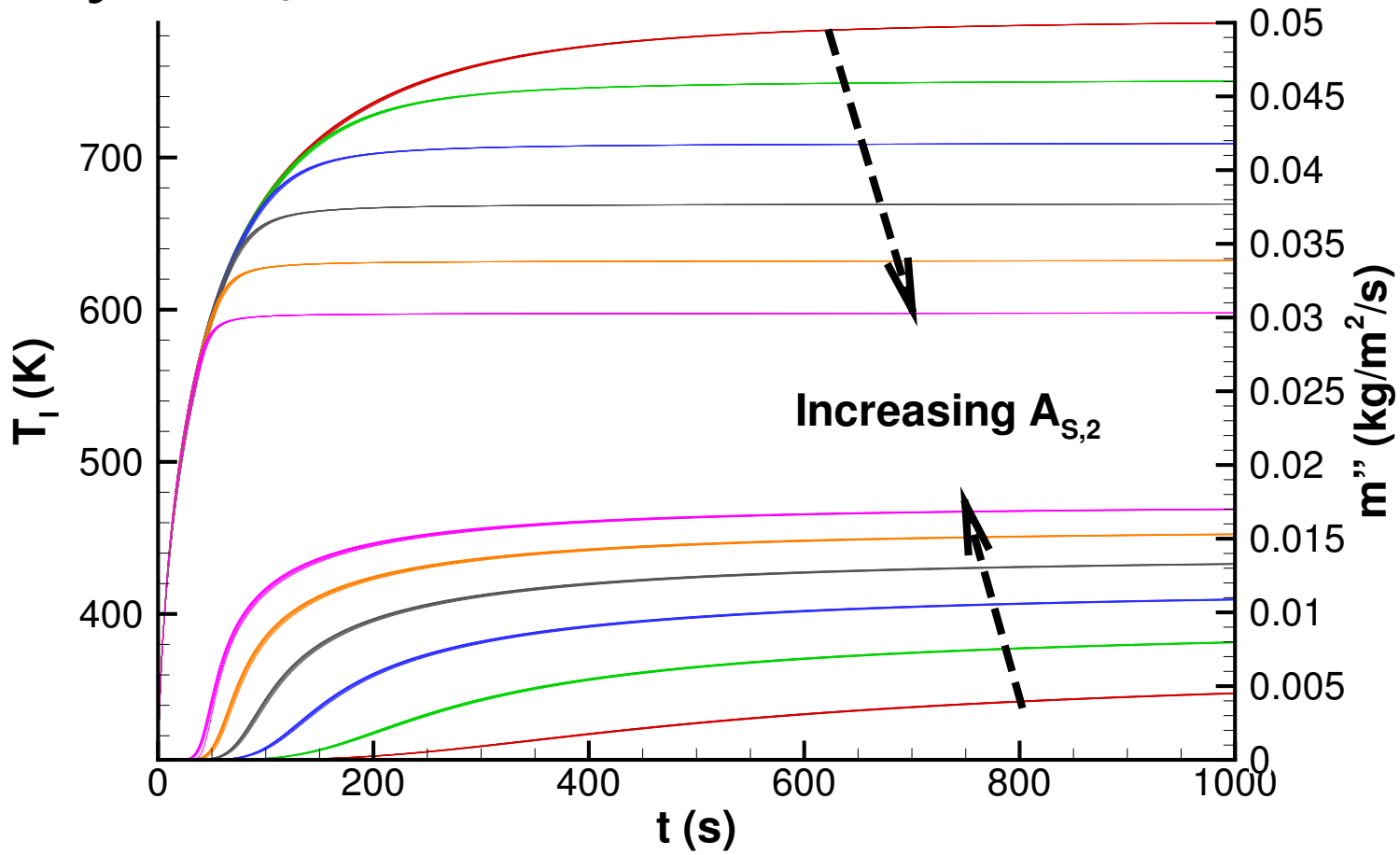


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2. A_S is varying.

- $A_{S,1}$ and $A_{S,2}$ vary from 10^{10} to 10^{15} s^{-1}
- No influence of $A_{S,1}$!
- Stabilization for large values of $A_{S,2}$
- Large mass loss rate $\Leftrightarrow$ low steady state interface temperature

Sensitivity to E_a

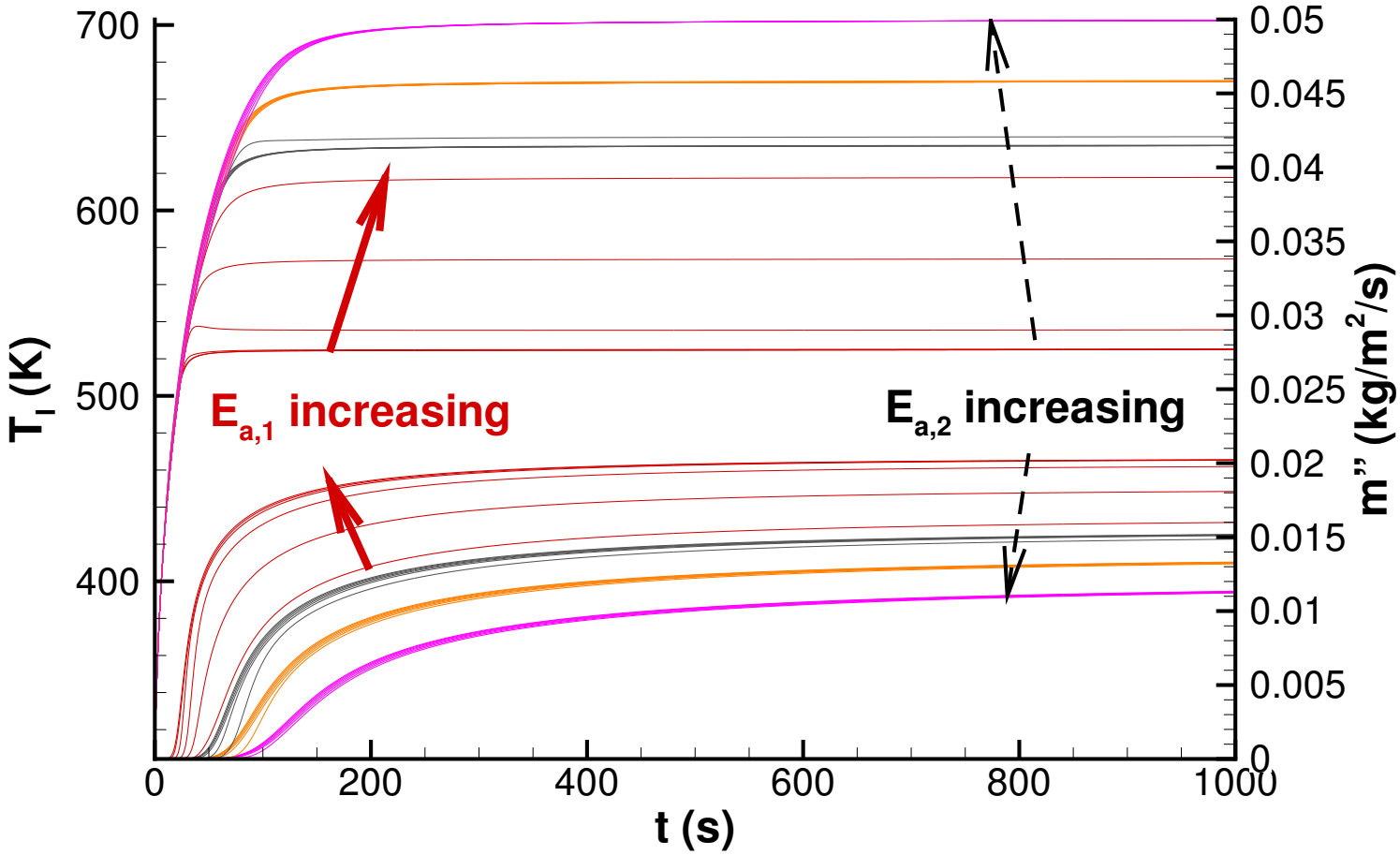


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2 for various activation energy values.

- $E_{a,1} \in [83, 139]$ kJ/mol;
- $E_{a,2}$: 145 kJ/mol (red lines) $\rightarrow$ 201 kJ/mol (purple lines)
- $E_{a,2} > 1.92\ 10^5$ kJ/mol $\Longrightarrow$ no dependence from $E_{a,1}$

Sensitivity to L_2

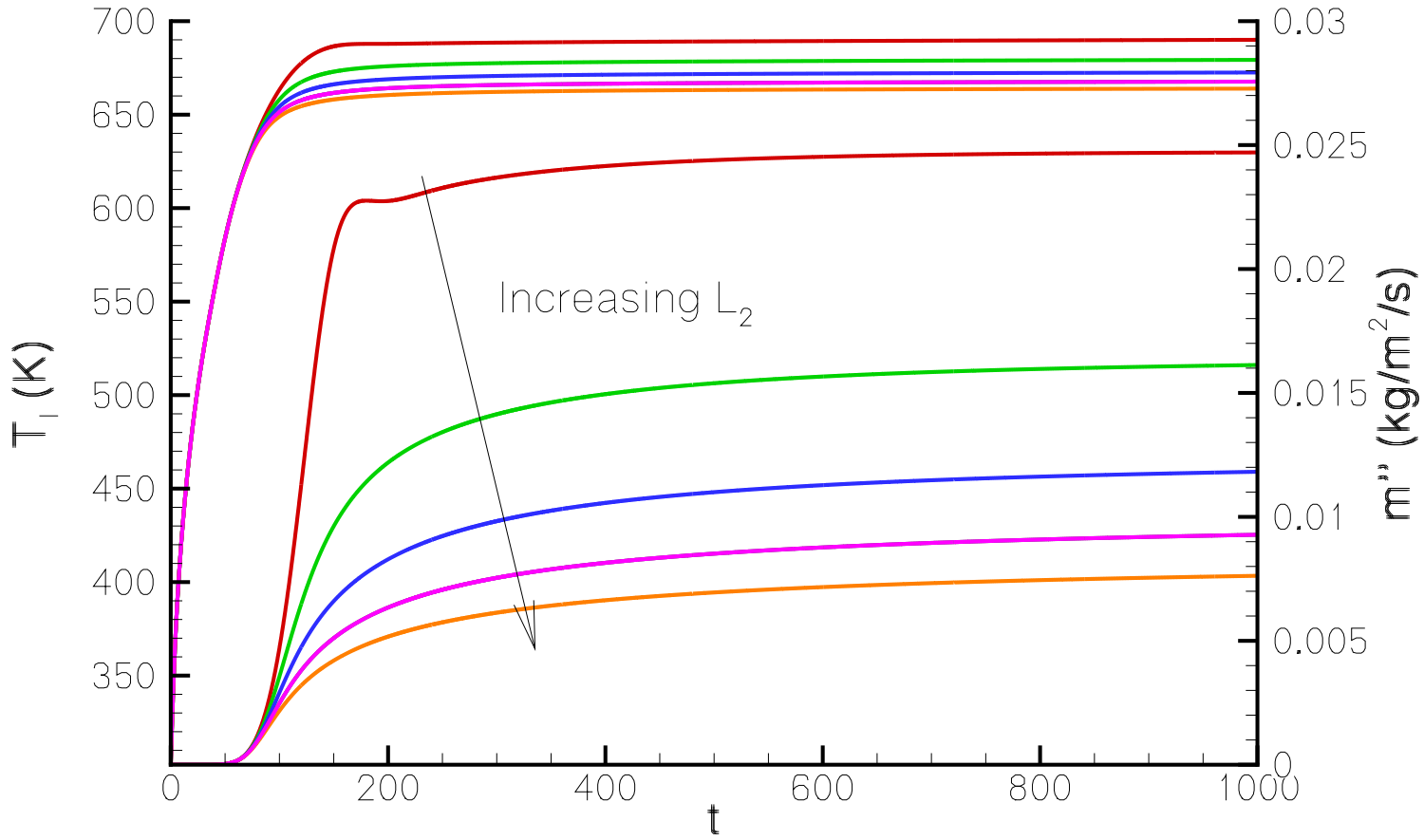


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2. Variations of the heat of pyrolysis.

- $L_2 \in [5\ 10^5, 3\ 10^6]$ J/kg

Sensitivity to h and ε

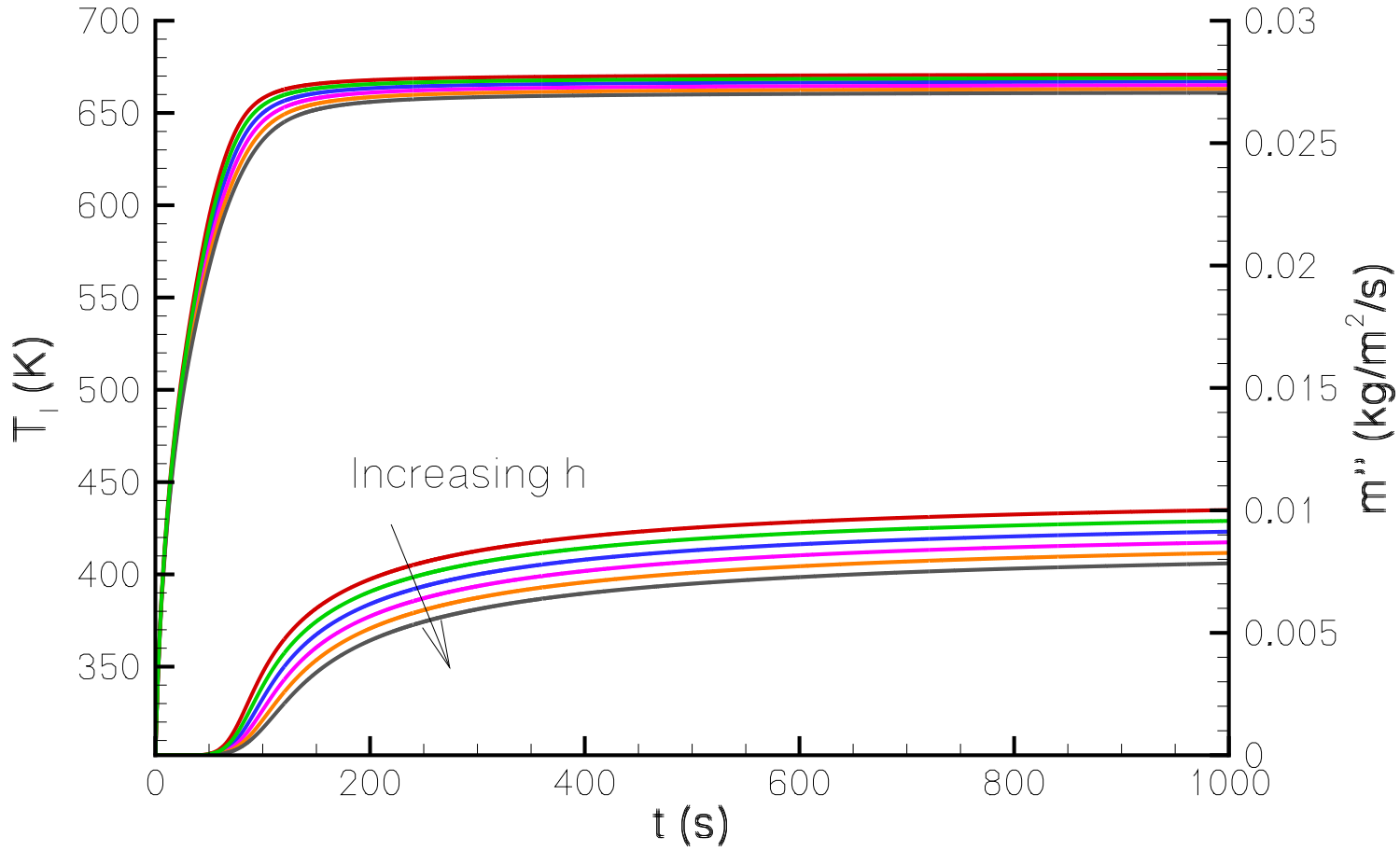


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2. Variations of the convective heat exchange coefficient.

- $h \in [5, 25]$ W/m/K, $\varepsilon \in [0.8, 1]$

Sensitivity to h and ε

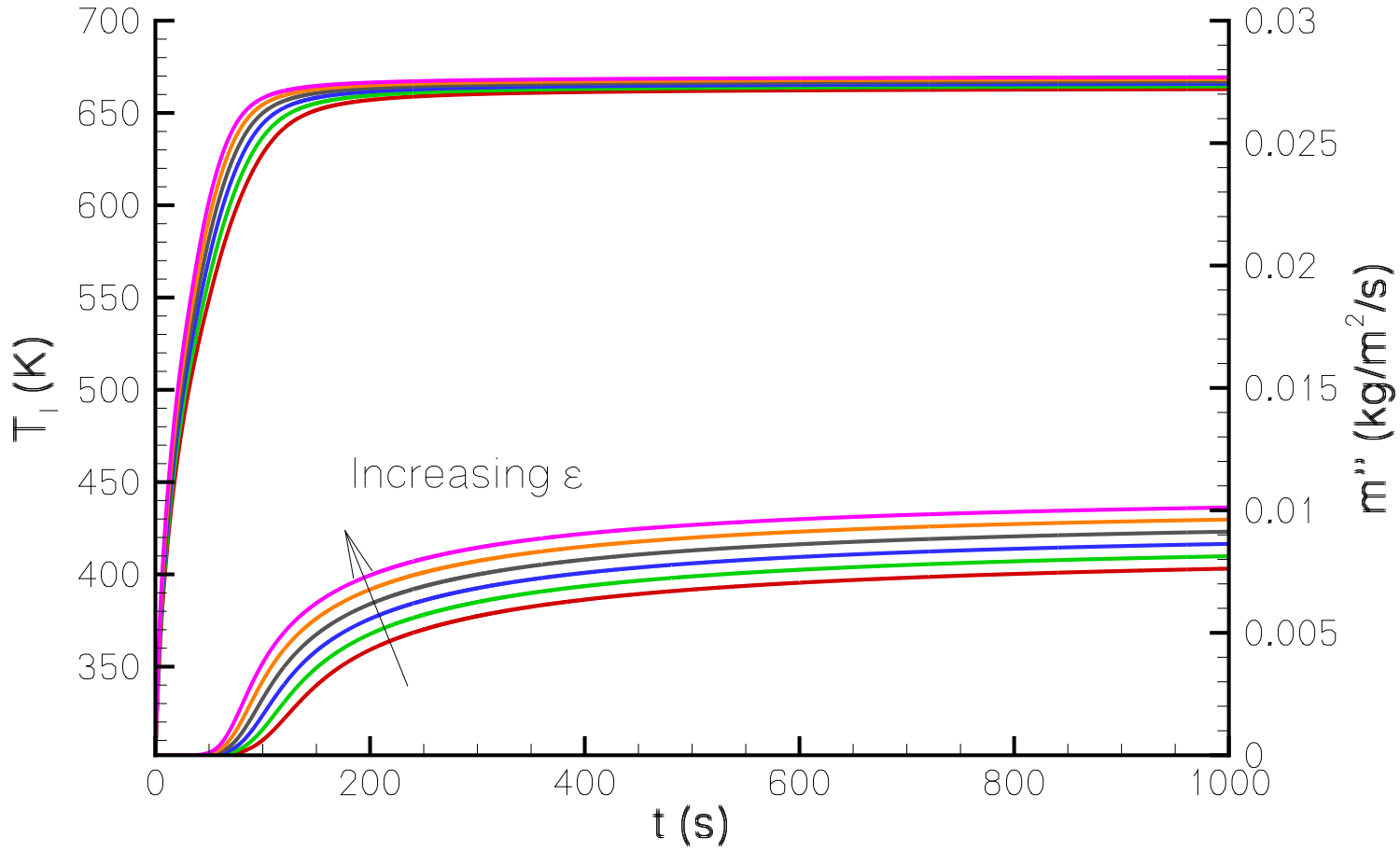


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2. Variations of the surface emissivity.

- $h \in [5, 25]$ W/m/K, $\varepsilon \in [0.8, 1]$

Sensitivity to h and ε

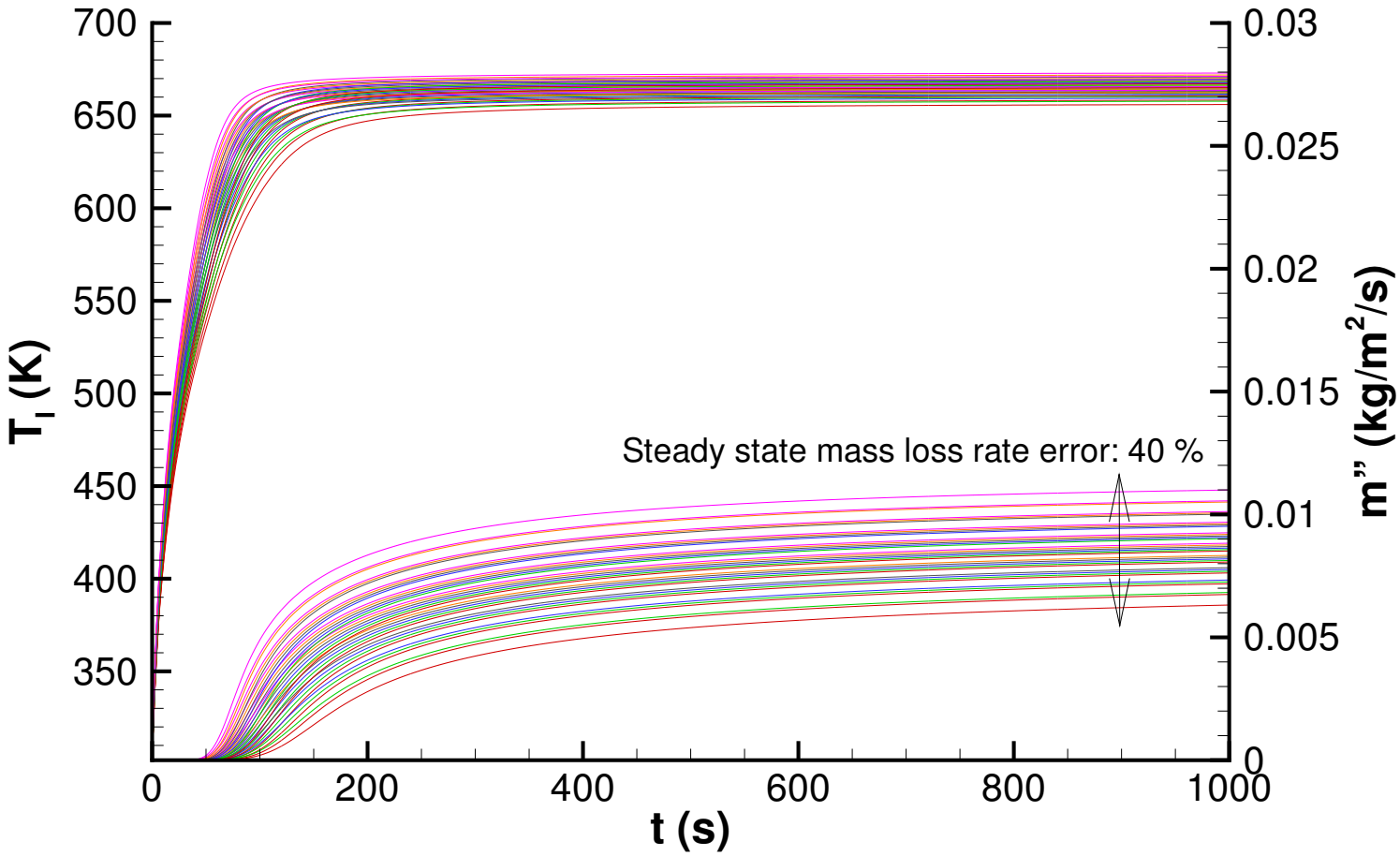


Figure : Interface temperature (T) and mass loss rate ($\dot{m}''$) computed for $\varphi_{\text{imp}} = 40$ kW/m^2. Both parameters varying.

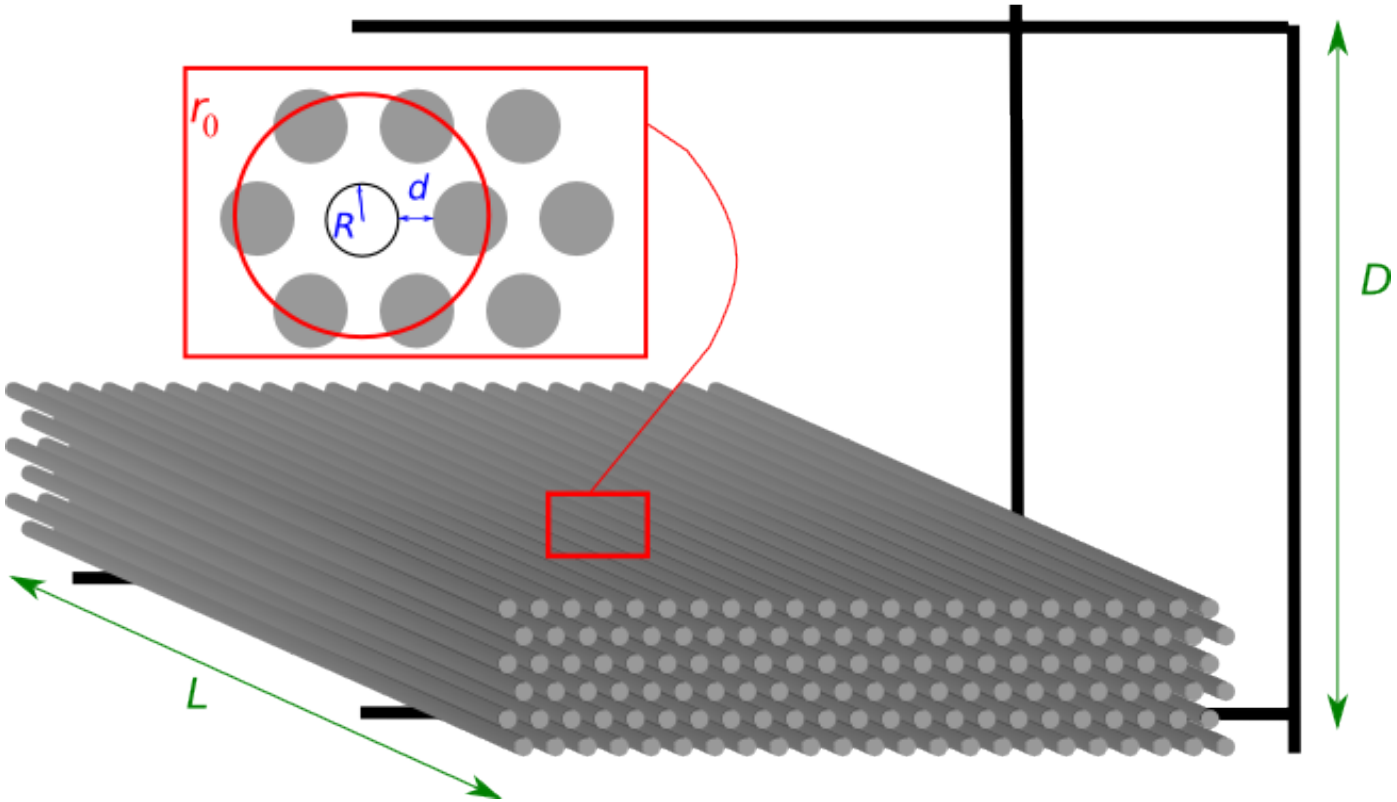
- $h \in [5, 25]$ W/m/K, $\varepsilon \in [0.8, 1]$

Outline

Cable tray modelling

Scale separation

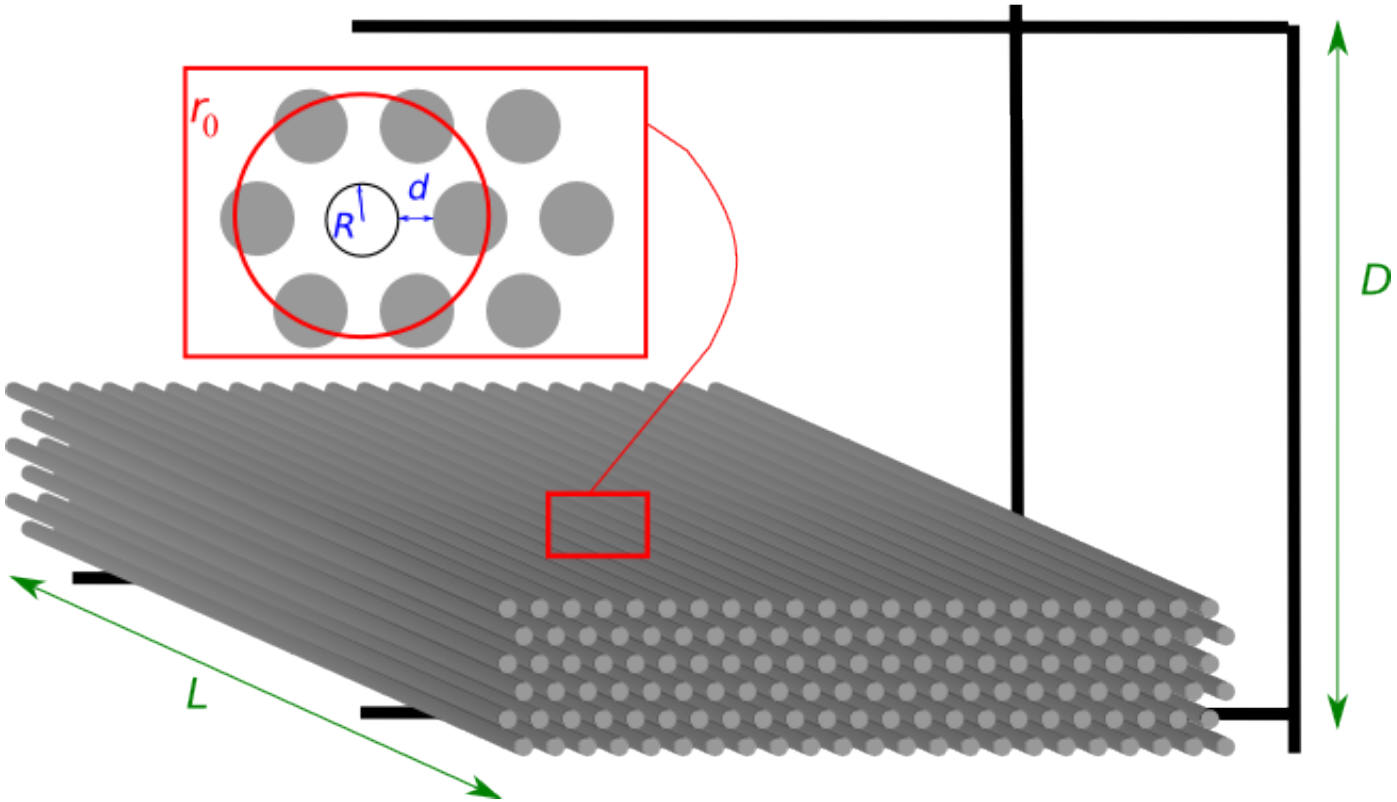
- Local scale: cable diameter R, distance between two cables d;



Cable tray modelling

Scale separation

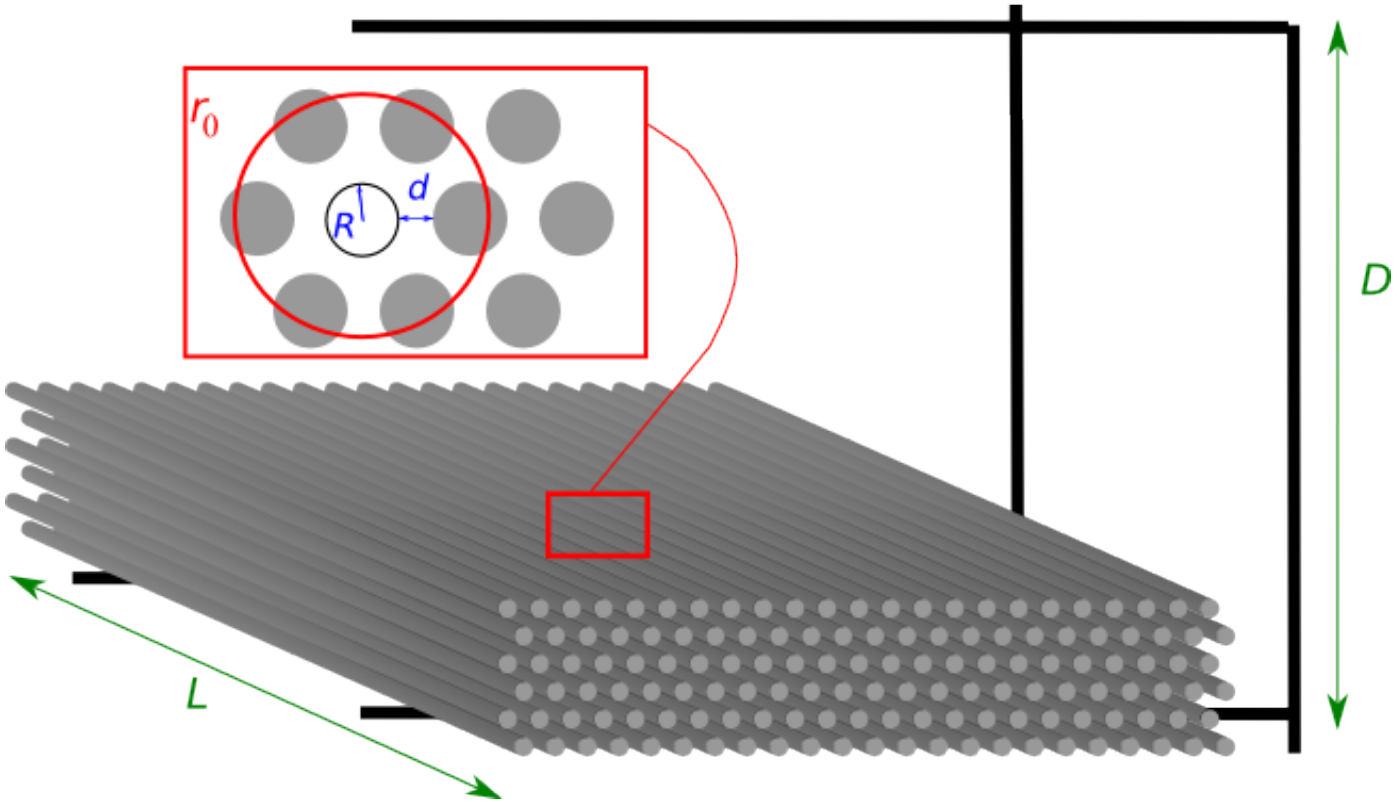
- Local scale: cable diameter R, distance between two cables d;
- Tray length scale L, distance between two trays D;



Cable tray modelling

Scale separation

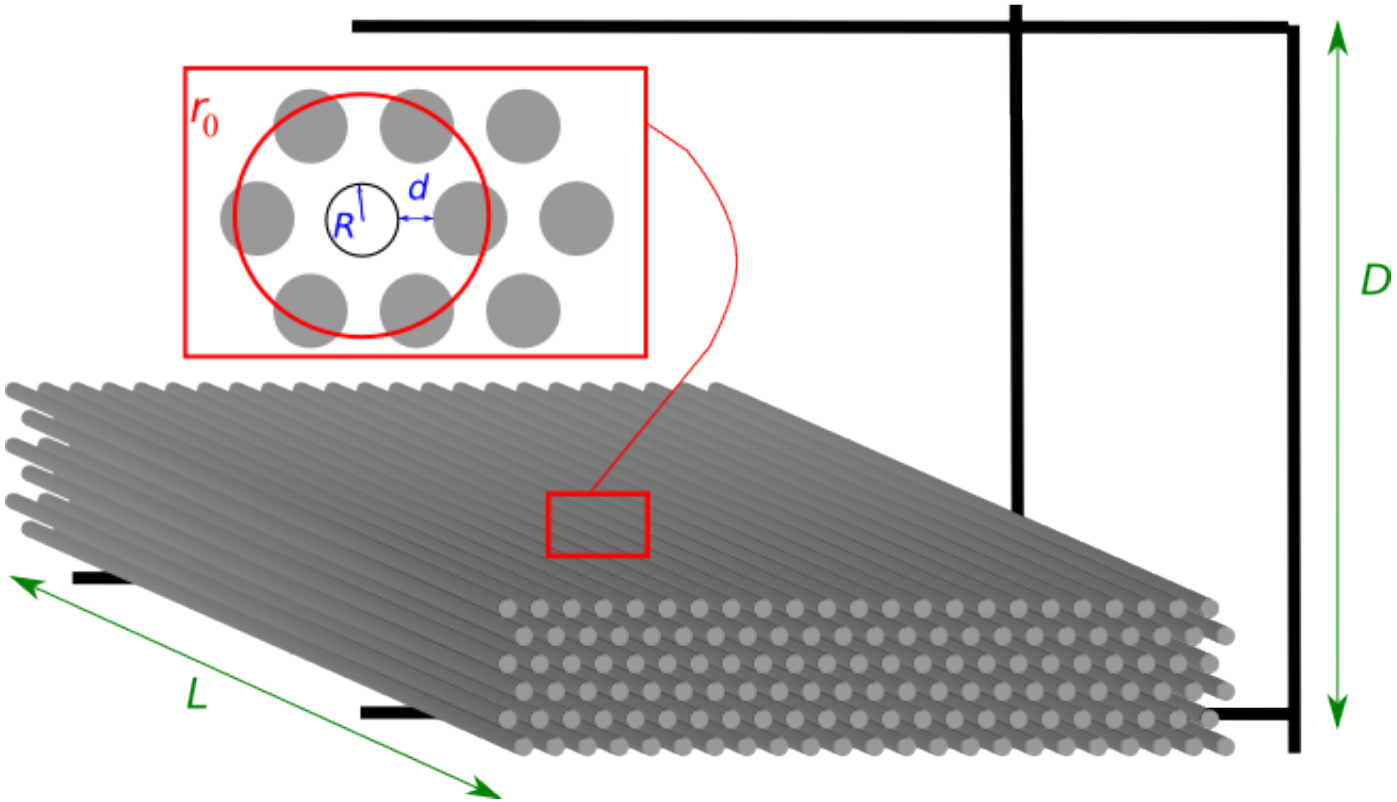
- Local scale: cable diameter R, distance between two cables d;
- Tray length scale L, distance between two trays D;
- *Homogeneisation* scale to be introduced r_0 (*representative volume element*)



Cable tray modelling

Scale separation

- Local scale: cable diameter R, distance between two cables d;
- Tray length scale L, distance between two trays D;
- *Homogeneisation* scale to be introduced r_0 (*representative volume element*)
- Separation assumption: $(R, d) \ll r_0 \ll (L, D)$



Homogeneization methods

- First step: using the current model with slight enhancements
  - 1D-modelling to 3D-modelling
  - convective effects in the cable tray modeled as a porous medium: addition of a Darcy law
  - associated convective heat transfers
- Important remark: the Darcy law $\Leftrightarrow$ basic homogeneization of the Navier-Stokes equations in porous media
- Second step: improved homogeneisation techniques
  - small scale "non-porous" pyrolysis model
  - homogeneization of the small scale model
  - the resulting closure model to be solved is specific of the cable tray configuration