

# Flame propagation in dust clouds: Euler-Lagrange simulations based on volume averaging method with closure

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## Background & Motivations

□ Context: Dust explosion hazard in nuclear safety analysis

➡ Decommissioning activities of UNGG reactors

Graphite/Magnesium mixtures -  $d_p \lesssim 100 \mu\text{m}$ ,  $\alpha_p < 10^{-3}$

➡ Loss of vacuum accident in the vessel of fusion reactors

Tungsten/Beryllium mixtures -  $d_p \lesssim 100 \mu\text{m}$ ,  $\alpha_p < 10^{-3}$

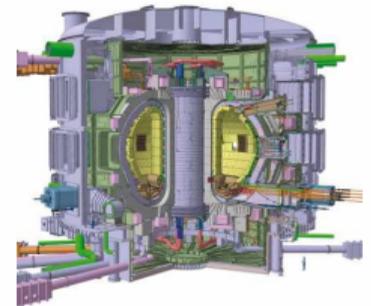
... Recurring situation in many other industrial installations: coal mines, cereal industry, ...



Tank farm accident - Blaye 1997



Natural Uranium Graphite Gas reactors (UNGG)



International Thermonuclear Experimental Reactor (ITER)

## Background & Motivations

- How to assess the risk ? As gaseous deflagrations ...
  - ⇒ Explosivity of dust clouds is first evaluated through "*intrinsic properties*"
    - Minimum ignition temperature,
    - Laminar flame speed  $s_L$ ,
    - ...
  - ⇒ Risk assessment tools use these properties as input parameters
    - Turbulent flame closure model [Peters, JFM 1999]
$$\frac{s_T}{s_L} = 1 + C \left( \frac{u_{rms}}{s_L} \right)^n$$
      - $0.5 \leq n \leq 1$  for gaseous mixtures
      - $n \sim 1$  for dust clouds [Sylvestrini *et. al*, J. Loss Prev. Process Ind. 2008]

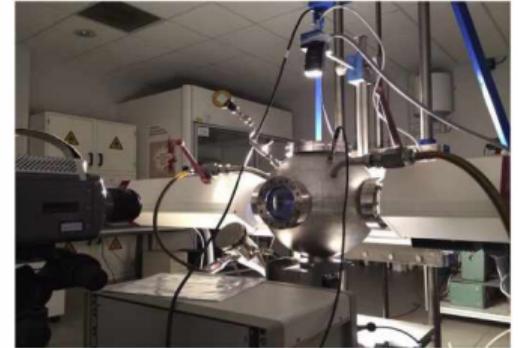
## Background & Motivations

□ How to evaluate *intrinsic properties* ? As gaseous deflagrations ...

⇒ Using normalized experiments

[D'Amico *et. al*, J. Loss Prev. Process Ind. 2016]

- Similar facilities: 20L spherical bomb, ...
- Additional difficulties: many parameters, induced or parasitic turbulence



⇒ Attempt to use DNS-like tools (CANtera, CHEMKIN, ...) to complete experiments

## Objectives

### □ Use of DNS-like simulations

- ➡ As a complementary tool to characterize explosion properties of dust clouds
- ➡ Through some of the most important *intrinsic properties*: laminar flame speed
- ➡ Acts as a pre-processor for turbulent flame speed closure models

### □ DNS-like simulations

- ➡ Fully resolved simulations are out of range: use of *macro-scale* Euler-Lagrange description
- ➡ Use of an up-scaling methodology
  - Provide a comprehensive methodology from the particle-scale to the macro-scale description
  - Get insights regarding the validity/limitations of the commonly used macro-scale models
- ➡ First estimate of the laminar flame speed for monodispersed graphite particles

## Outline

### **DNS-like simulations of flame propagation in dust clouds**

The Euler-Lagrange approach

Up-scaling methodology: the volume averaging method with closure

Macro-scale heat transfer: The lumped approximation and limiting behavior

Predicted macro-scale temperatures vs averaged DNS results

### **Application: flame propagation in graphite clouds**

Numerical set-up using CALIF<sup>3</sup>S-P<sup>2</sup>REMICS

Definition of the Representative Averaging Volume

From DNS to the laminar flame speed

## Perspectives

## Euler-Lagrange methodology for simulating flame propagation in dust clouds

### □ Euler-Lagrange description

⇒ Eulerian description of the carrier phase: up-scaling from point wise description

$$\partial_t \alpha \langle \rho \rangle + \nabla \cdot (\alpha \langle \rho \rangle \langle \mathbf{u} \rangle) = -\frac{1}{V} \sum_{p=1}^{N_V} \dot{m}_p$$

$$\partial_t \alpha \langle \rho \rangle \langle Y \rangle_k + \nabla \cdot (\alpha \langle \rho \rangle \langle \mathbf{u} \rangle \langle Y \rangle_k) = \nabla \cdot (\alpha \langle \rho \rangle \langle D \rangle_k \nabla \langle Y \rangle_k) + \langle \dot{\omega} \rangle_k - \frac{1}{V} \sum_{p=1}^{N_V} \dot{m}_{pk}$$

$$\partial_t \alpha \langle \rho \rangle \langle \mathbf{u} \rangle + \nabla \cdot (\alpha \langle \rho \rangle \langle \mathbf{u} \rangle \otimes \langle \mathbf{u} \rangle) = \nabla \cdot (\langle \boldsymbol{\tau} \rangle) + \alpha \langle \rho \rangle \mathbf{g} - \frac{1}{V} \sum_{p=1}^{N_V} \mathbf{f}_p$$

$$\partial_t \alpha \langle \rho \rangle \langle H \rangle + \nabla \cdot (\alpha \langle \rho \rangle \langle \mathbf{u} \rangle \langle H \rangle) = \nabla \cdot (\alpha \langle \lambda \rangle \nabla \langle T \rangle) + \langle \dot{\omega} \rangle_T - \frac{1}{V} \sum_{p=1}^{N_V} Q_p$$

⇒ Lagrangian description of the dispersed phase

$$d_t r_p = \rho_p A_p \dot{m}_p, \quad d_t \mathbf{x}_p = \mathbf{u}_p, \quad m_p d_t \mathbf{u}_p = \mathbf{f}_p + \rho_p \mathbf{g}, \quad (m C_p)_p d_t T_p = Q_p + \Delta H \dot{m}_p$$

### □ Issues

⇒ How to evaluate the coupling terms ?

⇒ How to define average quantities ?

## Up-scaling methodology based on volume averaging method with closure

□ A reduced representative problem: heat transfer in a dispersed two-phase system

⇒ Monodisperse rigid spherical particles, constant physical properties

⇒ Homogeneous heat source in the solid phase (mimic burning particles)

$$\text{in the } \beta\text{-phase: } \partial_t ((\rho c_p)_\beta T_\beta) + \nabla \cdot ((\rho c_p)_\beta T_\beta \mathbf{u}_\beta) = \nabla \cdot \lambda_\beta \nabla T_\beta$$

$$\text{in the } \sigma\text{-phase: } \partial_t ((\rho c_p)_\sigma T_\sigma) + \nabla \cdot ((\rho c_p)_\sigma T_\sigma \mathbf{u}_\sigma) = \nabla \cdot \lambda_\sigma \nabla T_\sigma + \omega_\sigma$$

$$\text{at } A_{\beta\sigma}: \quad T_\beta = T_\sigma \quad \text{and} \quad \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla T_\beta = \mathbf{n}_{\beta\sigma} \cdot \lambda_\sigma \nabla T_\sigma$$

□ Up-scaling methodology

⇒ Volume average over a Representative Averaging Volume of the continuous phase

⇒ Volume average over each particle of the dispersed phase

⇒ Closure consists in looking for an approximate solution for the deviations of  $T_\beta$

## Up-scaling methodology: (i) volume averaging

### □ Continuous carrier phase

⇒ Eulerian framework

⇒ Volume average over a REV of size  $r_0$  with  $d_p \ll r_0 \ll L$

$$\partial_t \left( \alpha_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \right) + \nabla \cdot \left( \alpha_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \langle \mathbf{u}_\beta \rangle^\beta \right) = \nabla \cdot \left( \mathbf{K}_\beta \cdot \nabla \langle T_\beta \rangle^\beta \right) - \frac{1}{V} \sum_{p=1}^{N_p} Q_{\beta p}$$

$$\text{where: } Q_{\beta p} = - \int_{A_p} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla T_\beta \, dS$$

### □ Dispersed phase

⇒ Lagrangian framework (requires  $x_p(t)$ )

⇒ Volume average over each particle

$$(m c_p)_p \frac{dT_p}{dt} = Q_{\beta p} + \omega_p V_p$$

## Up-scaling methodology: (ii) looking for an approximate solution

□ By introducing the decomposition  $T_\beta = \langle T_\beta \rangle^\beta + \tilde{T}_\beta$ , the macro-scale heat exchange reads:

$$Q_{\beta p} = - \int_{A_p} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \langle T_\beta \rangle^\beta dS - \int_{A_p} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \tilde{T}_\beta dS$$

⇒ This results in a mixed, macro micro-scale heat transfer problem, for  $\langle T_\beta \rangle^\beta$  and  $\tilde{T}_\beta$  !

⇒ From the micro-scale problem for  $\tilde{T}_\beta$ , an approximate solution can be sought by mapping  $\tilde{T}_\beta$  as:

$$\tilde{T}_\beta(\mathbf{x}, t) = - \sum_{p=1}^{N_V} s_p(\mathbf{x}) \left( \langle T_\beta \rangle^\beta \Big|_{x_p} - T_p \right)$$

⇒ The mapping variables  $s_p$  that realize an approximate solution are solution of *closure problems*

$$\lambda_\beta \nabla^2 s_p - \frac{\alpha_\beta^{-1}}{\mathcal{V}} \sum_{k=1}^N A_k h_{pk} = 0, \text{ in the } \beta\text{-phase}$$

$$s_p = 1, \text{ at } A_p$$

$$s_p = 0, \text{ at } A_k, \text{ with } k \neq p$$

$$\langle s_p \rangle^\beta = 0$$

## Up-scaling methodology: the resulting macro-scale model

$$\partial_t \left( \alpha_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \right) + \nabla \cdot \left( \alpha_\beta (\rho c_p)_\beta \langle T_\beta \rangle^\beta \langle \mathbf{u}_\beta \rangle^\beta \right) = \nabla \cdot \left( \mathbf{K}_\beta \cdot \nabla \langle T_\beta \rangle^\beta \right) - \frac{1}{V} \sum_{p=1}^{N_V} Q_{\beta p}$$

$$(m c_p)_p \frac{dT_p}{dt} = Q_{\beta p} + \omega_p V_p$$

□ Macro-scale heat exchange

⇒ Volume averaging with closure

$$Q_{\beta p} = - \int_{A_p} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla \langle T_\beta \rangle^\beta dS + \sum_{k=1}^{N_V} A_p h_{pk} \left( \langle T_\beta \rangle^\beta - T_k \right), \text{ with } h_{pk} = \frac{1}{A_k} \int_{A_k} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla s_p dS$$

⇒ Traditional approach - Undisturbed/locally disturbed isolated particle [Ling *et. al*, PoF 2016]

$$Q_{\beta p} = - \int_{A_p} \mathbf{n}_{\beta\sigma} \cdot \lambda_\beta \nabla T_\beta^0 dS + A_p h_p \left( T_\beta^0 - T_p \right)$$

↪ Similar form but  $\langle T_\beta \rangle^\beta$  and  $T_\beta^0$  refer to different quantities

↪ Additional particle-particle coupling terms

## Up-scaling methodology: lumped approximation and limiting behavior

### □ The lumped approximation

- ➡ Additional coupling terms increase the complexity of the macro-scale model
- ➡ The *a priori* calculation of effective coefficients represents a challenging task
- ➡ Interest in using a lumped approximation

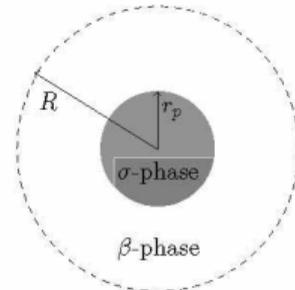
$$Q_{\beta p} = A_p h_p \left( \langle T_\beta \rangle^\beta - T_p \right) - \sum_{k=1}^{N_\gamma} A_p h_{pk} (T_k - T_p) \quad \text{with} \quad h_p = \sum_{k=1}^{N_\gamma} h_{pk}$$

### □ The Chang's unit cell [Chang, AIChE 1983]

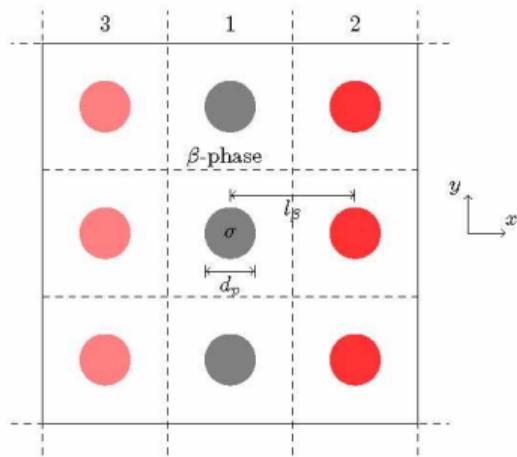
- ➡ Allows to obtain an analytical solution of the closure problems (perfect slip)

$$\frac{h_p d_p}{\lambda_\beta} = \frac{10\alpha_\beta^2}{9 \left( 1 - (1 - \alpha_\beta)^{1/3} \right) - \alpha_\beta (3 + \alpha_\beta)}$$

- ➡ Exhibits similar tendencies as those provided by empirical correlations
- ➡ Reduces to the classical value of 2 for the Nusselt number as  $\alpha \rightarrow 1$

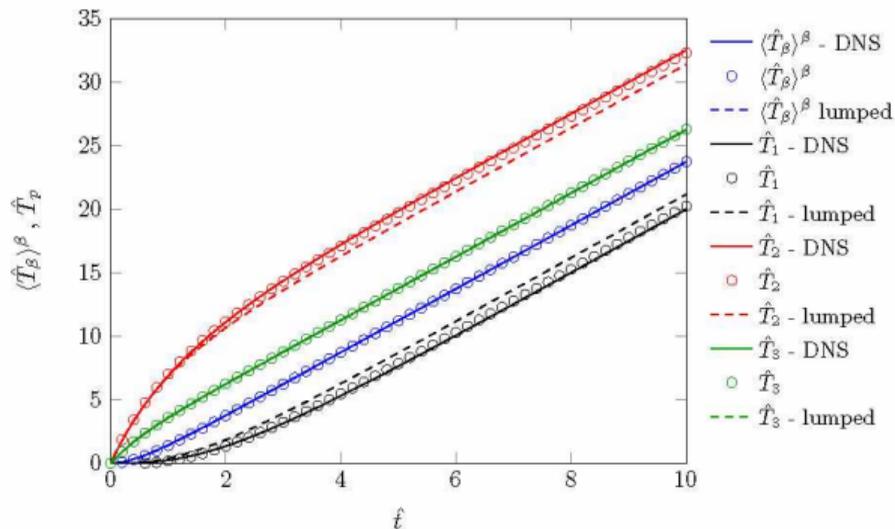


## Assessment of the macro-scale model and validity of the lumped approximation



3D micro-scale geometry - infinite in all directions

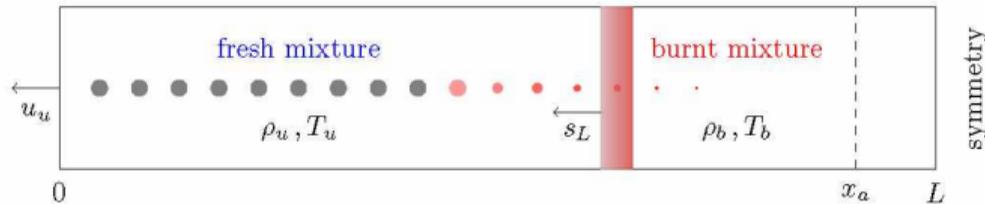
$\frac{\lambda_\sigma}{\lambda_\beta}$	$\frac{(\rho c_p)_\sigma}{(\rho c_p)_\beta}$	$\hat{\omega}_1$	$\hat{\omega}_2$	$\hat{\omega}_3$
$10^3$	$10^3$	0	10	5



- ➡ Predicted macro-scale temperatures are in good agreement with averaged DNS results
- ➡ The lumped approximation yields a good agreement for the carrier phase macro-scale temperature but temperature differences between particles are underestimated

## Application: flame propagation in graphite clouds and calculation of the laminar flame speed

- Numerical set-up: calculations using the open-source CALIF<sup>3</sup>S-P<sup>2</sup>REMICS CFD software



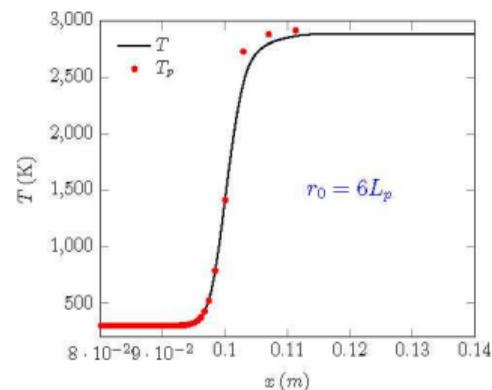
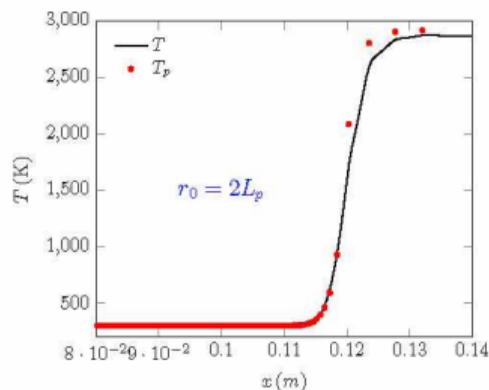
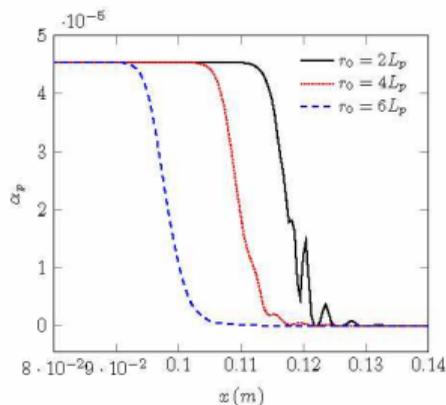
- ➡ One-dimensional like simulations with monodispersed graphite particles
- ➡ Initial inter-particles (and transverse) spacing:  $L_p = d_p \left( \frac{\pi}{6\alpha_p} \right)^{1/3}$
- ➡ One-step heterogeneous reaction:  $2C_{(s)} + O_2 \rightarrow 2CO$  (frozen homogeneous reaction)
- ➡ One-step homogeneous reaction:  $2CO + O_2 \rightarrow 2CO_2$  [Howard *et. al*, 1973]
- ➡ Ignition between  $x_a$  and  $L$  using a fictitious temperature in Arrhenius source terms

## Preliminary: On the choice of the Representative Averaging Volume

### □ Constraints on the size $r_0$ of the Representative Averaging Volume<sup>1</sup>

➡ To filter out micro-scale variations and ensure smoothness of averaged fields  $r_0 \gg d_p$

➡ To be able to describe macro-scale variations of averaged fields  $r_0 \ll L$

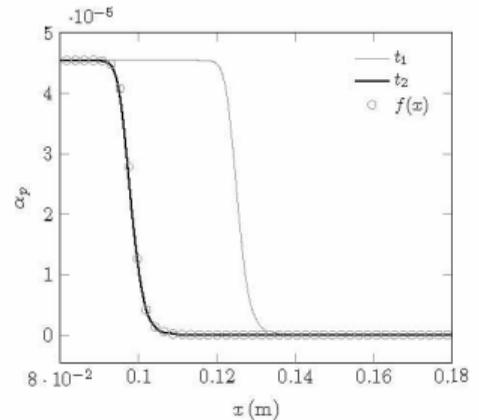
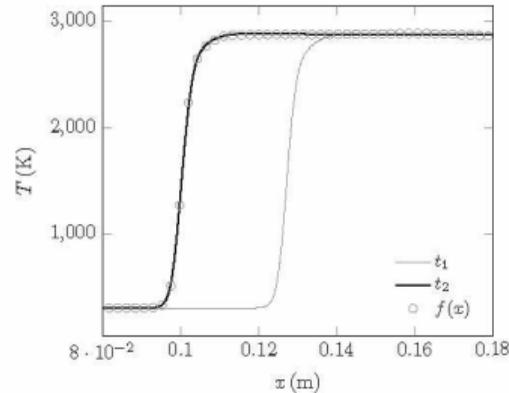
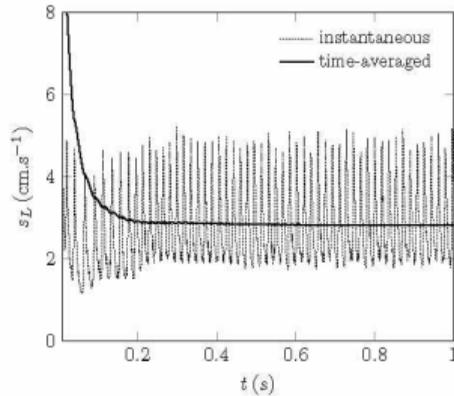


➡  $r_0 \geq 6L_p$  to ensure constraints

➡ Flame moves faster with  $r_0$ : effective diffusion

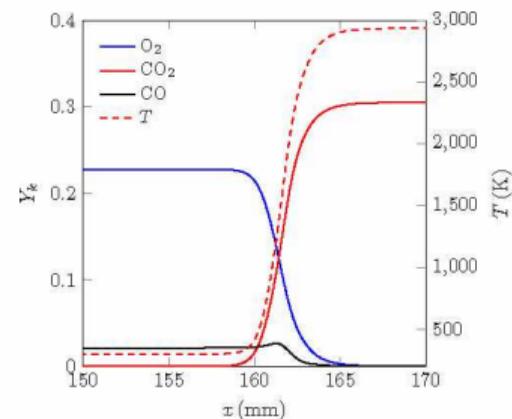
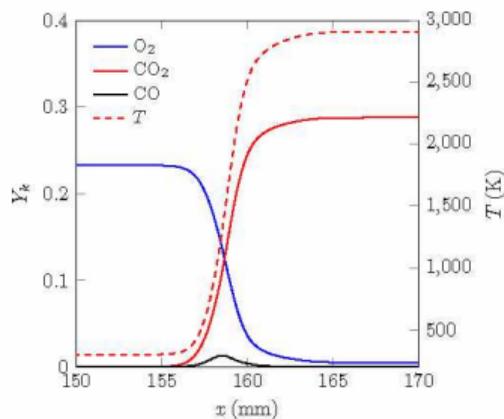
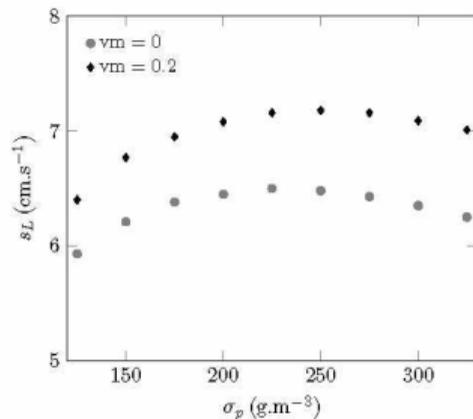
<sup>1</sup>In traditional approach, this issue is hidden in the mesh size and may conflict with mesh convergence

## From DNS to the laminar flame speed



- ➡ Instantaneous estimate  $s_L = \frac{\rho_b u_u - \rho_u u_b}{\rho_b - \rho_u}$
- ➡ After a short transient,  $s_L$  behaves as a quasi-periodic signal with mean  $\langle s_L \rangle$
- ➡ Period  $\sim$  distance between two successive particles by  $\langle s_L \rangle$  [Cloney *et. al*, Combustion & Flame 2018]
- ➡ Using  $s_a = \langle s_L \rangle + u_f$ , perfectly match the traveling wave assumption  $f(x) \equiv f(x - s_a(t_2 - t_1))$

## Preliminary results



➡ Access to the flame front structure and laminar flame speed

➡ Predicted laminar flame speed with different volatile content  $vm$  agrees with available experimental data [Ballal, Proc. Royal Soc. London, 1983]

## Perspectives

- Toward Euler-Lagrange simulations with metallic particles (work in progress):
  - Mass transfer: up-scaling for *attached flame* combustion regime
  - Heat transfer: up-scaling for radiative heat transfer
  
- Explosivity of dust clouds
  - Polydisperse and hybrid (graphite/metallic particles) effects
  - Access to additional *intrinsic properties*: lower flammability limits, ...