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A formalism for the estimation of the flame consumption speed for laminar spherical expanding flames

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Context & objectives

- Laminar Burning Velocity (LBV) noted S_l^0, is a fundamental flame property for combustion modeling and kinetic scheme improvement.
- LBV = Speed of fresh gases relative to the *1-D* stationnary laminar adiabatic **unstretched** flame front.

- In steady *1-D* geometry, LBV = consumption speed.
- In practice, LBV is often determined in Spherical Expanding Flame (SEF) configurations.
- Many strategies are used to define LBV in SEF configuration based on species consumption or on kinematics → results are different.

Goal of this work:

1. Propose a new methodology to determine the consumption speed in SEF configuration.
2. Develop a numerical tool to reproduce this configuration and validate this expression.

Laminar Burning Velocity definitions

S_l^0	Expression	Type	Remarks
1D Définitions:			
$S_{d,b}^0$	$S_{d,b}^0 = \frac{\rho_b}{\rho_u}(S_f^0 - U_b^0)$ [1,2]	Kinematic	Relative to burnt gases
$S_{d,u}^0$	$S_{d,u}^0 = S_f^0 - U_g^0$	Kinematic	Relative to Fresh gases
S_c^0	$S_c^0 = \frac{1}{\rho_u(Y_f^b - Y_f^u)} \int_{-\infty}^{+\infty} \dot{\omega}_f \; dx$ [3]	Kinetic	1D unstretched laminar flame
$\mathbf{1D} \Longrightarrow S_l^0 = S_{d,b}^0 = S_{d,u}^0 = S_c^0$			

How to determine the flame consumption speed?

The laminar flame speed definitions varie with the target species or the position of the flame front. Its definition is thus very ambiguous. Hereafter, a derivation of a model defines unambiguously the consumption speed.

S_c	Expression	Type	Remarks
Vélocity definitions for SEF:			
$S_{d,b}$	$S_{d,b} = \frac{\rho_b}{\rho_u}(S_f - U_b)$	Kinematic	Relative to burnt gases
$S_{d,u}$	$S_{d,u} = S_f - U_g$	Kinematic	Relative to fresh gases
S_c	$S_c = \frac{1}{-\rho_u Y_f^u R^2} \int_0^{R_0} \dot{\omega}_k r^2 \; dr$	Kinetic	SEF stretched flame speed for deficient species
$\mathbf{3D} \Longrightarrow S_i = S_l^0 - \mathfrak{L}_i.\kappa$ [3] $\Longrightarrow S_{d,b} \neq S_{d,u} \neq S_c$			

Consumption speed model

From conservation equations in a spherical confined volume combined with species and density transport equations:

$$\frac{\partial \rho Y_k}{\partial t} + \nabla.(\rho \mathbf{u} Y_k) = \nabla.(\rho D \nabla Y_k) + \dot{\omega}_k \quad \mathbf{(1)} \; , \qquad \frac{\partial Y_k}{\partial t} + \mathbf{S_f}.\nabla Y_k = 0 \quad \mathbf{(2)} \quad \text{and} \quad \frac{1}{\rho}\frac{\partial \rho}{\partial t} + \mathbf{S_f}.\frac{\nabla \rho}{\rho} = \frac{1}{\rho_u}\frac{d\rho_u}{dt} \quad \mathbf{(3)}$$

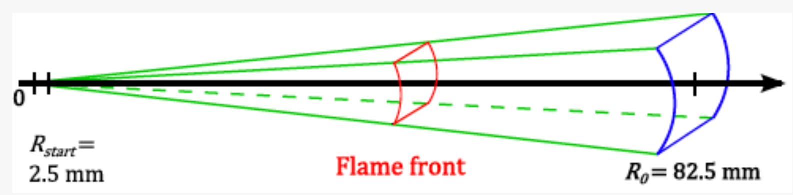
$$\langle S_c \rangle_{confined} = \underbrace{|S_f| \frac{(\rho_b Y_{f,b} - \rho_u Y_{f,u})}{\rho_u (Y_{f,b} - Y_{f,u})} + \frac{\rho_u Y_{f,u} R_0^3 + (\rho_b Y_{f,b} - \rho_u Y_{f,u}) R_{f,eq2}^3}{3 \rho_u (Y_{f,b} - Y_{f,u}) R_{f,eq}^2} \frac{1}{\rho_u}\frac{\partial \rho_u}{\partial t}}_{Kinematic} = \underbrace{\frac{1}{\rho_u (Y_{f,b} - Y_{f,u}) R_{f,eq}^2} \int_0^{R_0} (\dot{\omega}_f) \, r^2 dr}_{Kinetic} \quad (4)$$

With two radii definitions:

$$R_{f,eq} = \sqrt{\frac{\int_0^{R_0} (\rho Y_f - \rho_u Y_{f,u}) \, 2r dr}{(\rho_b Y_{f,b} - \rho_u Y_{f,u})}} \qquad \text{and} \qquad R_{f,eq2} = \sqrt[3]{\frac{\int_0^{R_0} (\rho Y_f - \rho_u Y_{f,u}) \, 3r^2 dr}{(\rho_b Y_{f,b} - \rho_u Y_{f,u})}} \quad \mathbf{(5)}$$

Numerical setup

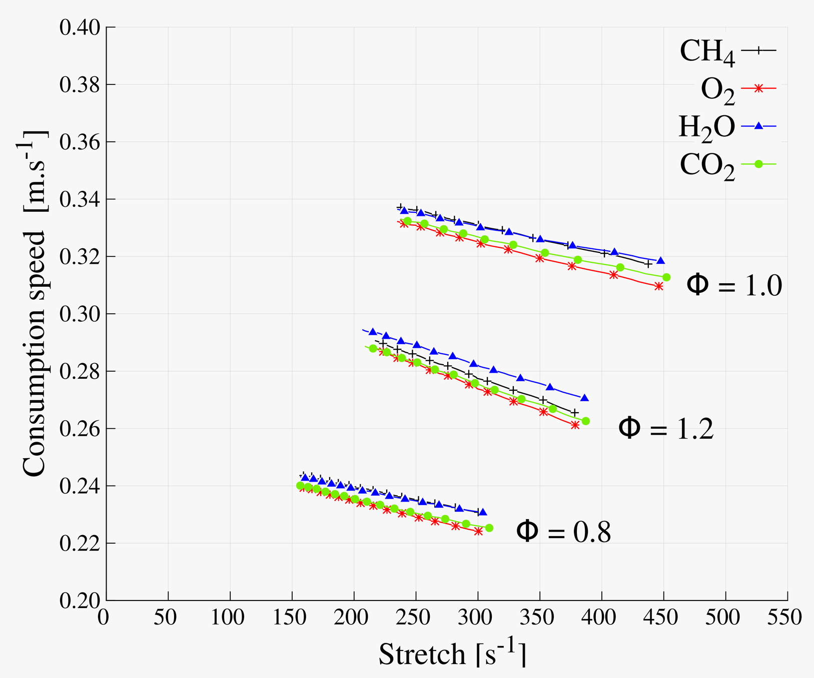
- Complex chemistry with kinetic scheme: GRI3.0 (53 species, 325 reactions)
- Unstructured adaptative meshes, [4, 5]
  - cell size = 10 µm,
  - number of elements = 4.1M .
- Aperture angle : 0.5°, L = 0.0825 m.



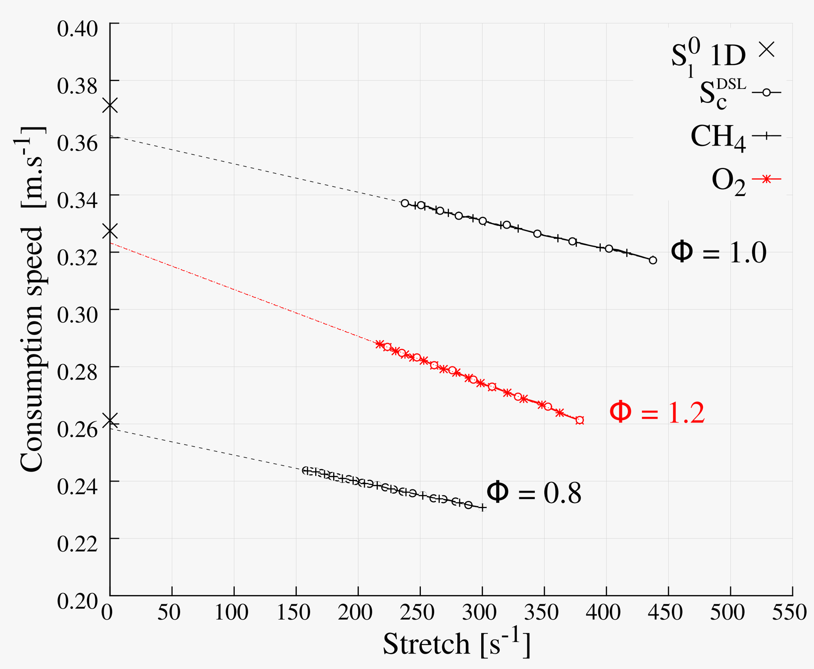
- Boundaries:
  - Periodic on the sides.
  - Walls in the radial directions.

Numerical results

The new Sc expression may be used for all major species

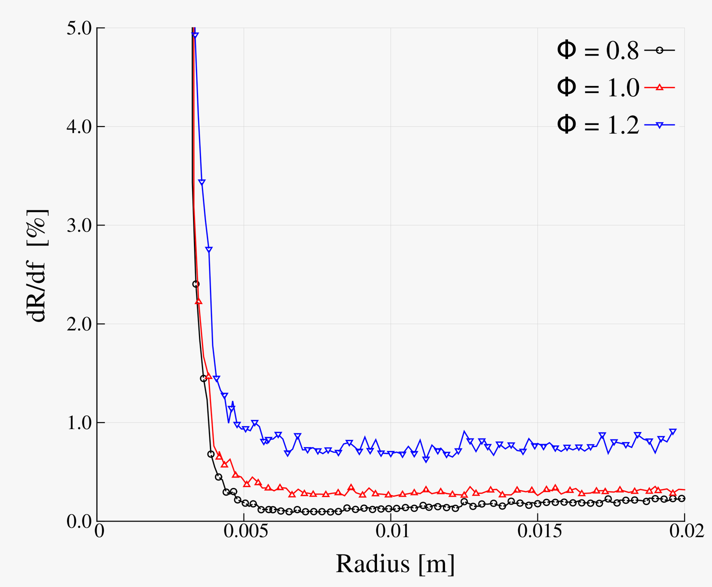


▲ Determination of the consumption speed with Eq. 4 LHS and RHS terms from several species for three different equivalence ratios of CH4/air flames at P = 1 atm and T = 300 K.



▲ Comparaison of Eq. 4 terms (LHS & RHS) calculated with the deficient reactive species for three different equivalence ratios of CH4/air flames.

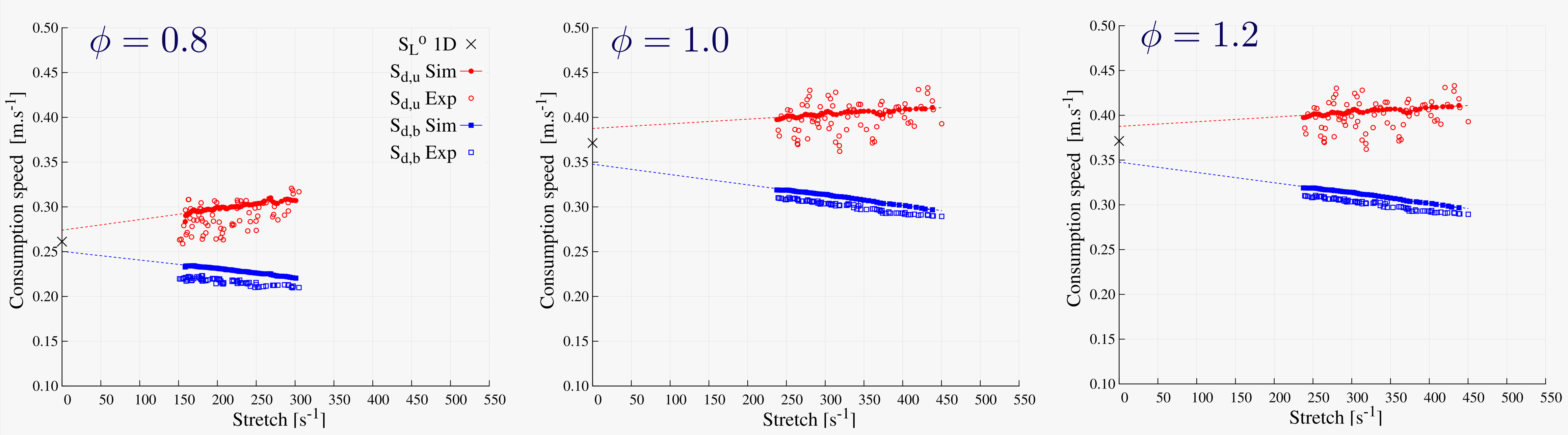
The radius difference $\boldsymbol{dR = |R_{f,eq} - R_{f,eq2}|}$ is small compared to the laminar flame thickness, (< 1 %).



▲ Evolution with the flame radius of the **dR** normalized by the flame thickness **df** for the three equivalence ratios of CH4/air.

Comparison of experimental & numerical results

Very good agreement with experimental data even for rich conditions.



▲ Comparaison between numerical and experimental data for velocities $S_{d,b}$ and $S_{d,u}$ of CH4/air flames.

Conclusion & perspectives

1. An unambiguous expression for the consumption speed in spherical expanding flame configuration.
2. Adaptation of the existing inhouse CFD code YALES2 and a new numerical setup able to reproduce with high fidelity real 3D spherical expanding flames.
3. Numerical results have validated our expression for CH4/air mixtures for all the major species.

Perspectives:

1. Explore other mixtures and thermodynamical conditions.
2. Use the derived equation **(4)** to mesure experimentally the flame consumption speed, Sc.

References

[1] *Bradley and al, Comb. Flame (26), 1996*
[2] *Varea et al., Comb. Flame (159), 2012*
[3] Poinsot & Veynante, Theoritical and numerical combustion, 3rd Ed
[4] *Moureau et al., C.R. Mecanique,2011*
[5] yales2.coria-cfd.fr