

# Temperature and pollution control in flames

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Controlling flame shapes and emissions is a major objective for all combustion engineers. Considering the complexity of reacting flows, novel optimization methods are required: this paper explores the application of control theory for partial differential equations to combustion. Both flame temperature and pollutant levels are optimized in a laminar Bunsen burner computed with complex chemistry schemes. The optimization procedure is coupled with mesh adaptation to provide grid-independent results. Finally, a recursive semi-deterministic global optimization approach is tested.

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## 1. Introduction

Control of temperature and species in flames is an important challenge for industrial and environmental issues. Many studies exist on numerical simulation of pollutant formation in flames (Peters & Donnerhack 1981; Warnatz 1981; Williams 1985; Pitsch *et al.* 1996; Poinso & Veynante 2001; Pitsch 2002). This paper is to apply control theory for PDEs (Lions 2003) to flames.

We focus on a laminar bunsen H<sub>2</sub>-Air flame simulated with detailed chemistry and multicomponent transport (Burman *et al.* 2004). We concentrate on the reduction of the Zeldovich-NO, also called thermal NO. This is the major NO source in a bunsen H<sub>2</sub>-Air flame. We also study the control of temperature distribution in flames, which is of importance in combustion engine design. Finally, we pay attention to the control of flame length at given fuel rate in the flow. These formulations are alternative approaches to consider pollutant control in flame (Peters & Donnerhack 1981) and also have natural applications in the design of combustion chambers.

To keep the computational cost low we test here if it is possible to use approximate state and sensitivity evaluations (Mohammadi & Pironneau 2001) during optimization. Once the optimization is achieved, the final design is a posteriori validated by accurate calculation. In this sense, different discretizations are used for the computation of the state and gradient, and an unstructured mesh adaptation strategy is applied to adapt the mesh to the solution during optimization process (Frey 2001; Frey & George 2001; Debiane 2004).

As the functionals are not necessarily convex, we use a new recursive semi-deterministic global optimization approach. This algorithm permits to escape from local minima but has a lower cost than a genetic algorithm (Goldberg 1989; Ivorra 2005) because the nondeterministic features of the approach have been reduced. Randomness is introduced only when the deterministic part fails. In addition, in cases where the algorithm fails, the construction can be used together with a genetic algorithm to improve population selection and reduce the size of the sampling needed.

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## 2. Semi-deterministic recursive optimization

Most deterministic minimization algorithms can be seen as discretizations of the following dynamical system (Attouch & Cominetti 1996; Mohammadi & Pironneau 2001; Mohammadi & Saiac 2002) where  $x$  denotes the vector of control parameters belonging to an admissible space  $\Omega_{ad}$ .  $\zeta$  is a fictitious parameter.  $M$  is a local metric transformation and  $d$  a direction in  $\Omega_{ad}$ .

$$\begin{cases} M(\zeta)x_\zeta = -d(x(\zeta)) \\ x(\zeta = 0) = x_0 \end{cases} \quad (2.1)$$

For example if  $d = \nabla J$ , the gradient of the functional, and  $M = Id$ , the identity operator, we recover the classical steepest descent method while with  $d = \nabla J$  and  $M = \nabla^2 J$  the Hessian of  $J$ , we recover the Newton method. Quasi-Newton methods can also be recovered using approximate Hessian definition (Vanderplaats 1990).

In this work, the following assumptions for our optimization problem are made (Ivorra 2005):

- H1:  $J \in C^1(\Omega_{ad}, \mathbb{R})$ .
- H2: the infimum  $J_m$  is known. This is often the case in industrial applications.
- H3: the problem is admissible: the infimum is reached inside the admissible domain:  $\exists x_m \in \Omega_{ad}, s.t. J(x_m) = J_m$ .
- H4:  $J$  is coercive (i.e.  $J(x) \rightarrow \infty$  when  $|x| \rightarrow \infty$ ).

We consider that system (2.1) has a solution if for a given  $x_0 \in \Omega_{ad}$ , we can find a finite  $Z_{x_0}$  such that  $J(x(Z_{x_0})) = J_m$ :

$$\begin{cases} M(\zeta)x_\zeta = -d(x(\zeta)) \\ x(0) = x_0 \\ J(x(Z_{x_0})) = J_m \end{cases} \quad (2.2)$$

This is an over-determined boundary value problem which can be solved using classical techniques for BVPs (e.g. shooting, finite differences,...). Because we are interested in constrained global optimization we prefer to express the condition at  $Z_{x_0}$  on the functional instead of its gradient. Indeed, in our context a first order optimality condition is usually not satisfied at the infimum.

This over-determination is an explanation of why we should not solve global optimization problems with methods which are particular discretizations of first order differential systems. We could use variants of classical methods after adding second order derivatives (Attouch & Cominetti 1996):

$$\begin{cases} \eta x_{\zeta\zeta} + M(\zeta)x_\zeta = -d(x(\zeta)), \\ x(0) = x_0, \quad \dot{x}(0) = \dot{x}_0, \\ J(x(Z_{x_0})) = J_m \end{cases} \quad (2.3)$$

To avoid introducing too much perturbation in the method, we consider, in practice,  $|\eta| \ll 1$ .

The over determination can be removed, for instance, by considering  $x_0 = v$  for (2.1) (resp.  $\dot{x}(0) = v$  for (2.3)) as a new variable to be found by the minimization of  $h(v) = J(x_v(Z_v)) - J_m$ , where  $x_v(Z_v)$  is the solution of (2.1) (resp. (2.3)) found at  $\zeta = Z_v$  starting from  $v$ .

The algorithm  $A_1(v_1, v_2)$  reads:

- $(v_1, v_2)$  given,

- Find  $v \in \operatorname{argmin}_{w \in \mathcal{O}(v_2)} h(w)$  where  $h(w) = J(x_w(Z_w)) - J_m$ , with  $x_w(Z_w)$  solution of system (2.1) found at  $\zeta = Z_w$  starting from  $w$ , and  $\mathcal{O}(v_2) = \{t\overline{v_1 v_2}, t \in \mathbb{R}\} \cap \Omega_{ad}$ .
- return  $v$

The line search minimization might fail. For instance, a secant method degenerates on plateau and critical points. In this case, we add an external level to the algorithm  $A_1$ , keeping  $v_1$  unchanged, and looking for  $v_2$  by minimizing a new functional  $h^2$  defined by  $h^2(v_2) = \min_{v_1} h(v_1, v_2)$  by algorithm  $A_1(v_1, v_2)$ .

This leads to the following two-level algorithm  $A_2(v_1, v_2^2)$ :

- $(v_1, v_2^2)$  given,
- Find  $v_2 \in \operatorname{argmin}_{w \in \mathcal{O}(v_2^2)} h^2(w)$  where  $h^2(w) = h(A_1(v_1, w))$  and  $\mathcal{O}(v_2^2) = \{t\overline{v_1 v_2^2}, t \in \mathbb{R}\} \cap \Omega_{ad}$ .
- return  $v_2$

The choice of initial conditions in this algorithm contains the non-deterministic feature of the algorithm. The construction can be pursued building recursively  $h^i(v_2^i) = \min_{v_1} h^{i-1}(v_1, v_2^i)$  using  $A_{i-1}(v_1, v_2^i)$ , with  $h^1(v) = h(v)$  where  $i$  denotes the external level. Mathematical background for this approach and validation on academic test cases and solution of nonlinear PDEs are available (Mohammadi & Saiac 2002; Ivorra & Mohammadi & Redont 2004; Ivorra 2005).

In practice, this algorithm succeeds if the trajectory passes close enough to the infimum (i.e. in  $B_\varepsilon(x_m)$  where  $\varepsilon$  defines the accuracy in the capture of the infimum). This means that we should consider for  $h$  a functional of the form

$$h(v) = \int_{T_1}^T (J(x_v(\tau)) - J_m)^2 d\tau, \quad \text{for } 0 < T_1 < \tau < T$$

where  $x_v(\tau)$  is the trajectory generated by (2.1) and  $T_1 = T/2$  for instance. Also, in the algorithm above,  $x_w(Z_w)$  is replaced by the best solution found over  $[0, Z_w]$ .

In cases where  $J_m$  is unknown, we set  $J_m = -\infty$  and look for the best solution for a given complexity and computational effort. This is the approach adopted here where we predefine the effort we would like to make in each level of the algorithm.

### 3. Functionals and parameterizations

The symbols of this section are illustrated on figure (1), which shows the computational domain  $\Omega$ . A section  $\Gamma$ , through which we would like to reduce the NO flux, is defined at  $z = 1.5\text{cm}$ .

Optimization control parameters are:

- the inflow velocity of the premixed mixture  $v_1$  taken as

$$v_1(\overline{v_1}, p_1, p_2) = \overline{v_1} (1 - \exp(-\frac{|r_0 - r|}{r_1})) + S(p_1, p_2) \text{ with } r_0 = 0.2, r_1 = 0.05$$

with

$$S(p_1, p_2) = p_1 (\frac{r}{r_0})^{1.2} \sin(p_2 r) \sin(\frac{r - r_0}{r_0})$$

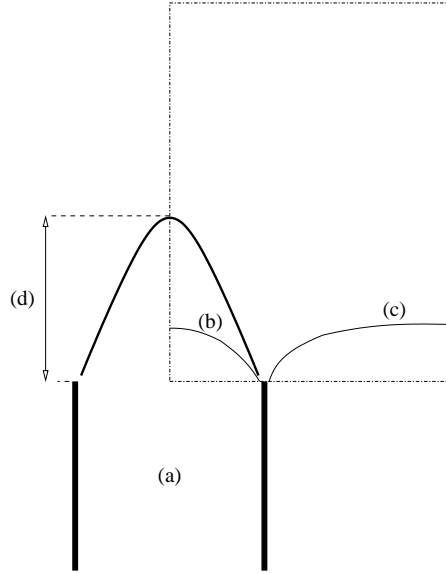


FIGURE 1. Computational domain for the bunsen flame and illustration of the parameterizations: (a) is the premixed mixture  $H_2$ ,  $O_2$ ,  $N_2$  injected with velocity  $v_1$  shown on (b), the coflow velocity  $v_2$  (c) and the length of the flame (d).

- the coflow velocity  $v_2$  of the form

$$v_2(\bar{v}_2) = \bar{v}_2 \left( 1 - \exp\left(\frac{-|r_0 + r_3 - r|}{r_1}\right) \right) \text{ with } r_3 = 0.05$$

Two of the following molar fraction quantities:

- the molar fraction of species  $H_2$  in the premixed mixture  $\chi_{H_2}$ ,
- the molar fraction of species  $O_2$  in the premixed mixture  $\chi_{O_2}$ ,
- the molar fraction of species  $N_2$  in the premixed mixture  $\chi_{N_2}$ ,

the third one being deduced from  $\chi_{H_2} + \chi_{O_2} + \chi_{N_2} = 1$

The control space has therefore six degrees of freedom. We introduce two nondimensional numbers:

- $\phi$ , the equivalence ratio, defined by:

$$\phi = \frac{\chi_{H_2} / \chi_{O_2_{inj}}}{(\chi_{H_2} / \chi_{O_2})_{stoich}} = \frac{\chi_{H_2}}{2\chi_{O_2}}$$

where *inj* means injection and *stoich* means stoichiometric.

- $\alpha = \frac{\chi_{N_2}}{\chi_{O_2}}$ , the dilution factor.

The vector of control parameters is  $x = (\bar{v}_1, p_1, p_2, \bar{v}_2, \phi, \alpha) \in [50, 200] \times [-25, 25] \times [-10, 10] \times [50, 200] \times [4, 10] \times [0, 10]$ . It should be noticed that a constraint on the fuel rate in the flow implies a compatibility relation between  $p_1, p_2$  and  $\bar{v}_1$ .

The first cost function we consider aims to reduce the NO flux through  $\Gamma$  and at the same time achieve a target temperature profile:

$$J_1(x) = \gamma_1 \int_{\Gamma} \rho y_{NO} v \cdot n + \gamma_2 \int_{\Gamma} (T - T_{target})^2$$

where  $\rho$  is the density,  $y_{NO}$  the mass fraction of NO,  $v$  the flow velocity,  $T$  the temperature

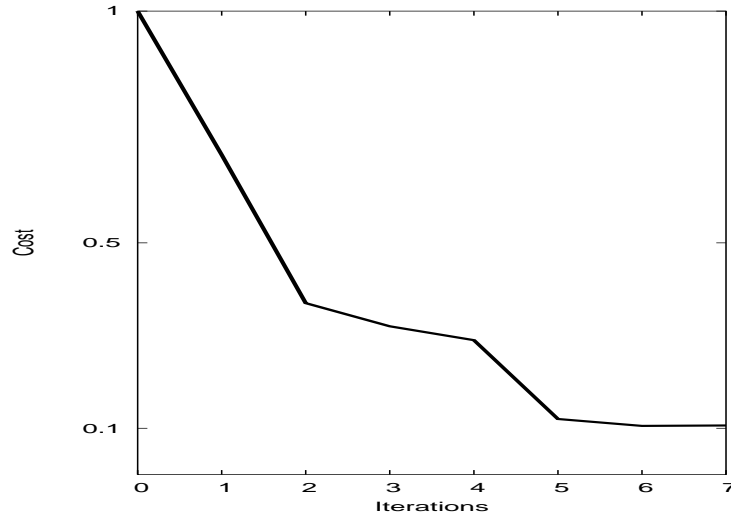


FIGURE 2. NO reduction functional  $J_1$  evolution vs. accumulation of optimization iterations. The two-level algorithm permits to escape from local minima: a first plateau is reached in first level and the second level permits to reach a second plateau with a global reduction of 90 percent in the functional while the original algorithm alone (i.e. with only one level) only leads to 60 percent reduction in the functional.

and  $T_{target}$  a target temperature profile.  $\gamma_1$ ,  $\gamma_2$  are given positive scalars and  $n$  the normal unit vector to  $\Gamma$ .

The second cost function aims to control the flame length at a given flow rate:

$$J_2(x) = \int_{r=0} y_{H_2} \quad \text{with} \quad \gamma_1 \int_{z=0} \rho y_{H_2} v \cdot n = \text{const.}$$

We observed that these functionals are not necessarily convex (Debiane 2004).

#### 4. State equations

The hydrogen mechanism can be described using nineteen elementary reactions and nine species  $H_2$ ,  $O_2$ ,  $H$ ,  $O$ ,  $OH$ ,  $HO_2$ ,  $H_2O$ ,  $H_2O_2$ ,  $N_2$ . The flame is simulated with an axisymmetric bunsen laminar flame code (Ern & Giovangigli 1994; Burman *et al.* 2004). Governing equations are discretized by a finite element method, which is an extension to chemically reacting flows of the streamline diffusion method, including least squares stabilization of the pressure gradient and the low-Mach continuity equation as well as a shock capturing term designed to control temperature and species mass fraction undershoots near flame fronts. The species  $NO$  and  $N_2$  are added to the mechanism in order to simulate the formation of the Zeldovich-NO (Williams 1985).

#### 5. Numerical results

As combustion computations are quite expensive, we will analyze the feasibility of incomplete state and sensitivity evaluation during optimization with intermediate accurate validation of the optimal configurations. This means that during optimization we mostly achieve suboptimal search and analysis (Mohammadi & Pironneau 2001). This is possible because the semi-deterministic algorithm above requires less accuracy in sensitivity

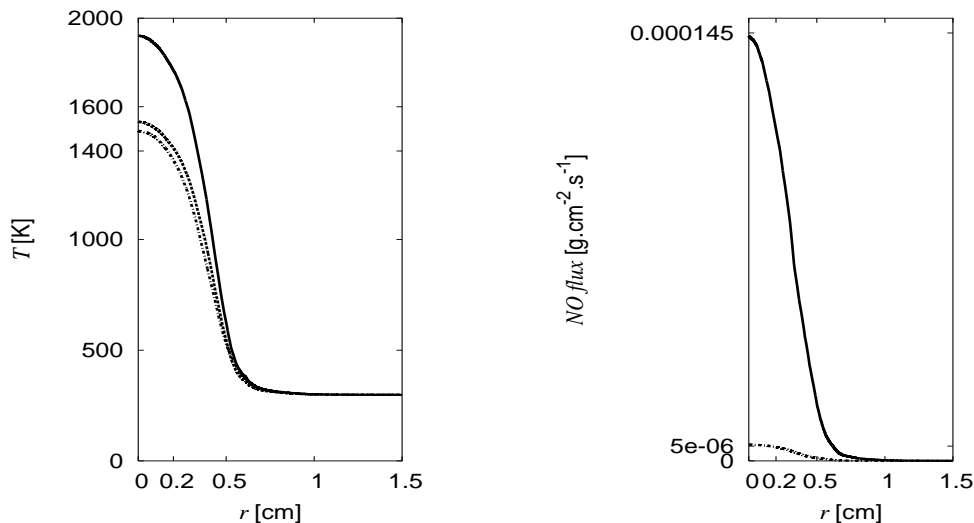


FIGURE 3. Left: initial (upper curve), target (lower) and optimized (middle) temperature profiles (K) along  $z = 1.5\text{cm}$  ( $r$ -axis in cm). Right: NO flux ( $\text{g}\cdot\text{cm}^{-2}\cdot\text{s}^{-1}$ ) through  $z = 1.5\text{cm}$  before (upper curve) and after (lower) optimization. The NO flux has been drastically reduced and the temperature target almost achieved.

definitions. Also, during intermediate sensitivity and state analysis the previous states are used to define a suitable initialization for the solver. In addition, gradient computations are made on a coarser mesh than the one used for state evaluations. On the other hand, to monitor the accuracy of state calculations, and therefore the functional, at each iteration of optimization an unstructured solution-based mesh adaptation is performed (Frey & George 2001; Frey 2001; Debiante 2004). Using these ingredients, the cost for optimization is only 30 percent of the overall flame calculations.

The optimizations shown here have been performed with two levels of the algorithm presented above. The effect of each level can be seen in figure 2: a first plateau is reached and the algorithm permits to reach a second plateau with a global reduction of 90 percent in the functional.

Optimization results for functional  $J_1$  are shown in figure 3. We can see that the target temperature is almost achieved and that the NO flux is drastically reduced. Initial and final temperature and NO mass fraction distributions are shown in figure 4.

Optimization results for functional  $J_2$  are shown in figure 5. We show the maximum and minimum flame lengths which can be obtained with the current parameterization. There is a difference of 30 percent in flame length between the two configurations. Figure 6 shows a Delaunay type adapted mesh based on solution-based metric control which permits to monitor numerical errors during simulation and optimization. The injection profiles obtained from maximizing and minimizing the flame length at a given flow rate are quite counter-intuitive (see Figure 7) as the maximum injection along the symmetry line leads to a minimum flame length. The explanation of this phenomenon, which requires more investigations, is probably linked with the diffusion of the dihydrogen. This optimization clearly shows the correlation between flame length and pollutant production.

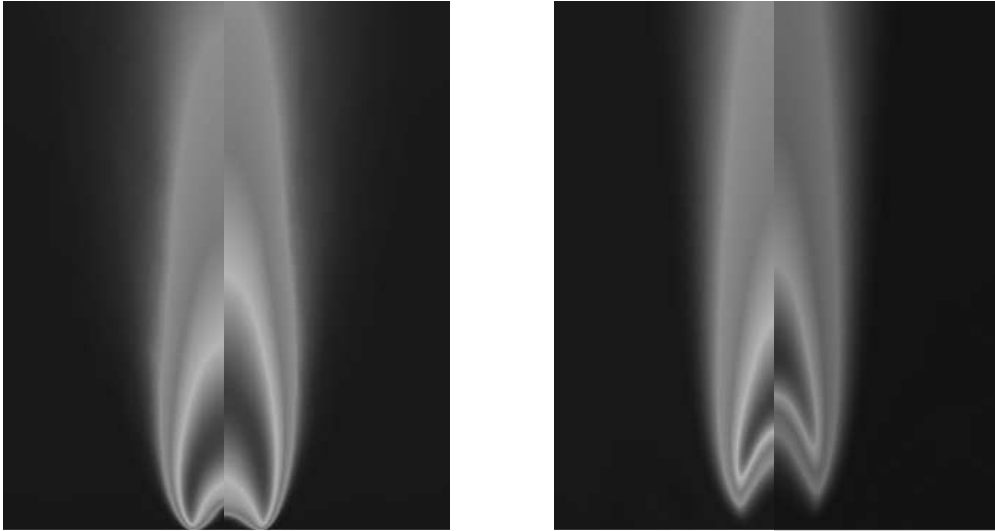


FIGURE 4. *Optimized and initial temperature (left) and NO mass fraction (right) distributions.*

## 6. Conclusions

A global optimization algorithm, based on the solution of boundary value instead of initial value problems, has been applied to the control of pollution, temperature and flame length in a bunsen flame simulated with complex chemistry making the problem stiff. It has been shown that controlling the fuel rate and the velocity profiles in both the premixed flow and the coflow is enough to achieve the targeted temperature, NO flux and flame shapes. Future investigations will concern shape optimization for such configurations in order to impact the design of combustion chambers.

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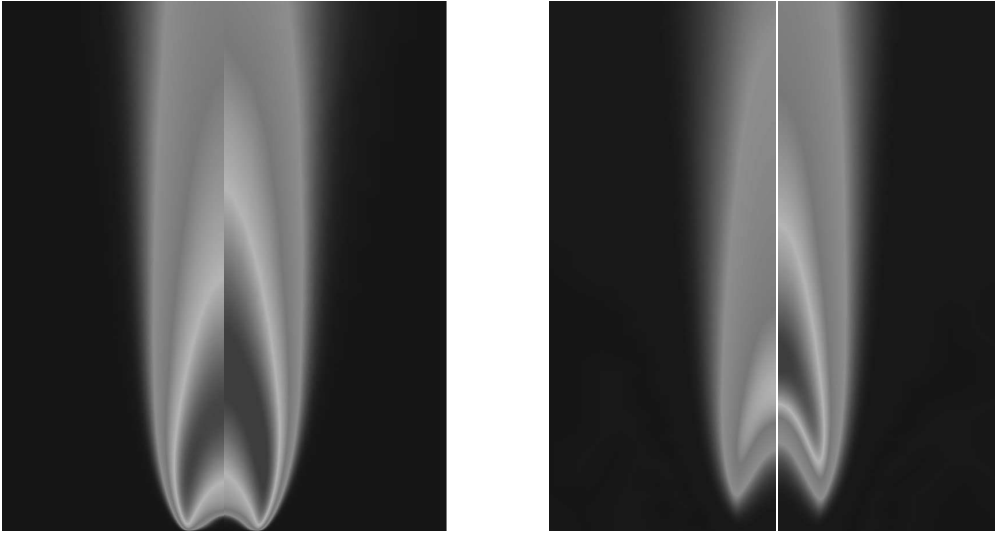


FIGURE 5. *Temperature contours (left) and NO mass fraction contours (right). There is a clear correlation between flame length and NO production.*

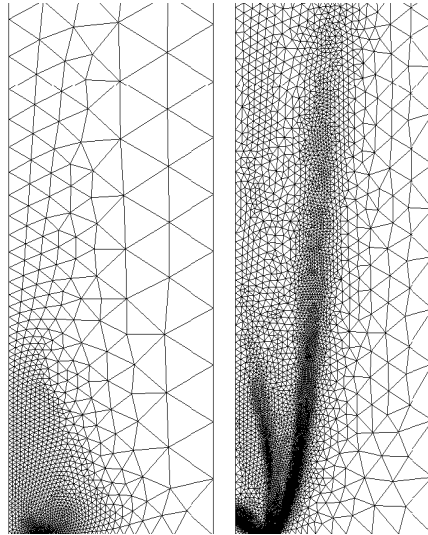


FIGURE 6. *Initial mesh (left) and adapted mesh (right). Solution-based adapted meshes permit to control numerical accuracy of the simulation and optimization.*

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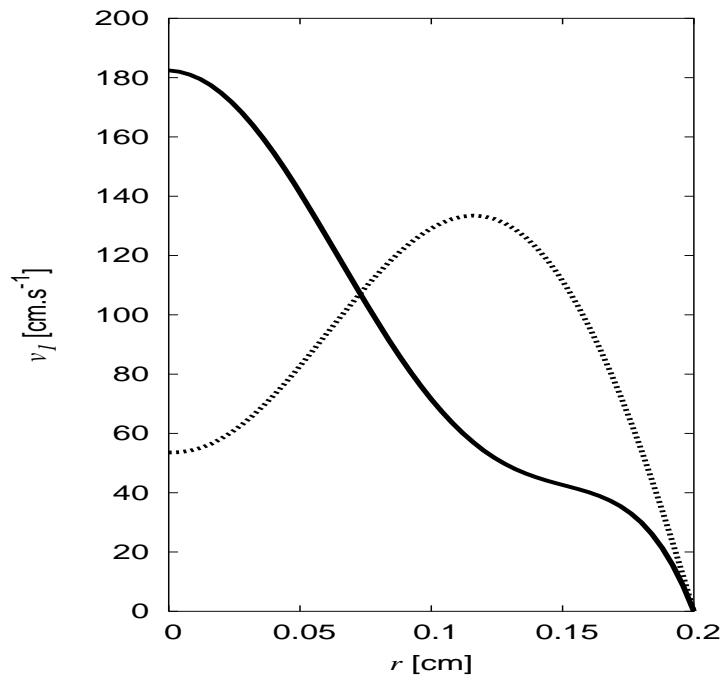


FIGURE 7. The injection velocity ( $\text{cm s}^{-1}$ ) profiles are quite counter-intuitive ( $r$ -axis in  $\text{cm}$ ) as the maximum injection along the symmetry line leads to a minimum flame length. The continuous profile minimizes the length of the flame and the dash profile maximizes it.

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