

## An approach for including evaporation in a model for predicting spray penetration

Gautham Krishnan\*, Narendiran C G\* and Shamit Bakshi  
Department of Mechanical Engineering,  
Indian Institute of Technology, Madras.  
Chennai - 600036, India.

### Abstract

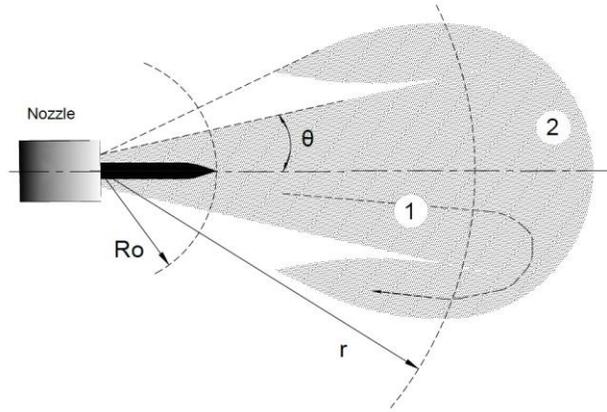
Fuel sprays have been a key topic of research in the field of IC engines, as it influences the efficiency and emission and hence the performance of the engines. But it is fairly tasking to deduce an exhaustively descriptive model of spray mechanics, because of the complexity of the physics involved and the number of parameters that affect the spray, which includes unsteady in-chamber conditions, phase change in the spray and the internal flow in the injector. Nevertheless many models with modest assumptions have been proposed, which reasonably capture the physics of fuel spray. The approach of fuel being considered as *isolated droplets* travelling in the spray and subsequent *evaporation effects* have been studied by a few. It has been thought that the effect of evaporation is negligible in many cases. In this work, we shall examine the mechanics using a fundamental approach and observe how droplet evaporation could affect the temporal evolution of high speed fuel spray in a pressurized chamber. An earlier model based on differential control volume analysis for the mass and momentum conservation of fuel and entrained ambient gas, is extended to account for the evaporation of the droplet.

**Keywords:** evaporative droplet spray, atomization, drop size, penetration length.

---

\*Corresponding author: gauthamkrishnan1996@gmail.com

\*Corresponding author: cgnarendiran@gmail.com



**Figure 1.** Schematic: Sketch of the propagating spray. Region 1 corresponds to the region of the steady radial expansion; Region 2 represents the tip of the spray. (Figure adapted from Roisman et al. [1])

## 1. Introduction

Several models, numerical and semi-empirical, describing the penetration of dense sprays exist in literature. These analyses [2,3] have been pursued by solving overall mass and momentum conservation equations for the multiphase flow in the propagating spray. Further analysis, owing to the fact that a jump condition in fluid properties exists at the front end of a spray has also been performed in analytical models of non-evaporating sprays [1].

It is known that the sprays develop vortex like ring structures at the front end. This is due to the prevailing conditions at the front end of the spray plume originating from the inertia of the ambient gas in front of the propagating spray and the jump conditions (volume fraction of the fuel change suddenly over a very short length to zero). Among other factors, spray penetration is also known to depend on the geometry of the spray nozzle and internal flow. Since we do not seek to incorporate these factors directly in the proposed model, we have to use at least one adjustable parameter to account for these effects. For this purpose, we shall use the breakup length ( $R_0$ ) of the spray and the corresponding droplet radius ( $r_{d0}$ ). A relationship between the penetration length and the time elapsed since spraying is computed numerically using the model and its variation

with the evaporation constant ( $k$ ) is studied and compared with few existing results. Both convective and diffusive types of evaporation can be considered in this model.

## 2. Theoretical Model

There exists a region of dense fuel core near the nozzle of the spray. Within this region it is assumed that no ambient gas is entrained and hence volume fraction of the fuel is unity here. At the end of this region, the fuel cone splits into  $N$  number of droplets at the breakup length,  $R_0$  (this depends on the nozzle diameter, cone angle and the volume fraction at breakup,  $\gamma_0$ ). The droplet number density ( $n$ ) is defined as the number of fuel droplets per unit volume. After the initial breakup of the dense spray into a large number of droplets, we assume that no further splitting of droplets or coalescence among the droplets occurs. Also, the front end of the spray is considered to be far enough from the nozzle at any instant that the details of the flow near the nozzle (dependent on nozzle geometry and internal flow) do not influence the penetration of the spray tip. Hence, the model is valid for penetration distances much greater than  $R_0$ .

After the breakup length, in the region 1 shown in Fig.1, the spray propagates radially outward. Many experimental studies have shown that spray propagation follows a conical shape in this region with a nearly constant cone half angle ( $\theta$ ). Droplet diameter ( $D$ ), droplet and entrained ambient gas velocity and volume fraction of fuel are assumed to be invariant in the azimuthal direction, and hence are functions only of the radial coordinate ' $r$ ' measured from the apex of the cone, coincident with the spray nozzle. This aids us in creating a one dimensional mathematical formulation describing the mechanics of the multiphase flow in the spray. In the performed analysis, the spray is also assumed to be wide enough so that the velocity of the entrained air is negligible further outside the cone of the spray [4]. The effect of evaporation of fuel droplets is introduced through the  $D^2$  law of evaporation [5]. Effectively this reduces the droplet diameter as it propagates and thus influences the mass and momentum balances.

The values of different parameters used for the simulation is listed in Table 1.

Parameters:	Symbols:	Representative values:
Total pressure inside the chamber	$P$	25 bar
Temperature inside the chamber	$T$	450 K
Density of the fuel	$\rho$	555 kg/m <sup>3</sup>
Fuel Saturation pressure	$P_{sat}$	6.61 bar
Nozzle Diameter:	$D_{nozzle}$	0.0001 m
Breakup length:	$R_0$	0.31 mm
Cone angle:	$\alpha$	25°
Volume ratio of fuel to ambient gas:	$\gamma_0$	0.311
Density of ambient gas	$\rho_a$	13.36 kg/m <sup>3</sup>
Fuel Velocity at breakup:	$u_0$	450 m/s
Initial Droplet Radius:	$r_{d0}$	25 * 10 <sup>-6</sup> m
Entrained gas Velocity at breakup:	$v_{a0}$	45 m/s
Effective Binary Diffusivity	$D_{ab}$	2 * 10 <sup>-6</sup> m <sup>2</sup> /s
Convective evaporative constant	$k_{conv}$	10 <sup>-5</sup> m <sup>2</sup> /s
Diffusive evaporative constant	$k_{diff}$	10 <sup>-7</sup> m <sup>2</sup> /s
Schmidt number	$Sc$	0.97
Reynolds number	$Re$	18000

**Table 1.** Various parameters and their representative values

### 3. Mathematical Formulation

#### a. Near Nozzle Region

Usually the geometry of the nozzle has a definite impact on the spray penetration. As proposed by Roisman et al. [1], in this model it has been accounted for by the breakup length ( $R_0$ ). This quantity has been also utilized as the scaling parameter for the non-dimensionalization of the spray penetration length. Since the Weber number of the droplets created is high, the energy involved in their formation is negligible in comparison with the kinetic energy of the spray at breakup. Hence we may safely assume that the velocity of the fuel at breakup is equal to that at injection

$$u_0 = u_i$$

Now from the conservation of mass of fuel:

Mass flux at nozzle:

$$u_i \frac{\pi D_{nozzle}^2}{4} = u_0 \gamma_0 \Omega r R_0^2$$

where the solid angle,

$$\Omega = 2\pi(1 - \cos \theta)$$

Therefore, the breakup length is given by,

$$R_0 = \frac{D_{nozzle}}{\sqrt{8\gamma_0(1 - \cos \theta)}}$$

At breakup length, the initial and maximum possible volume fraction of the liquid phase consisting of individual droplets is taken as  $\gamma_0 = 0.311$  [1, 6, 7, 8].

#### b. Conical Region of Radial Expansion

The following formulation holds true for the region of steady radial expansion i.e., region-I as defined by Roisman et al. [1].

Now consider a stationary differential control volume at a distance  $r$  from the nozzle (taken as origin) with  $dr$  as the thickness of the control volume, along  $r$ .

Therefore volume of the differential CV is given by,

$$\Delta V = \Omega r^2 dr$$

The volume fraction of the fuel (liquid phase) at  $r$ ,  $\gamma(r)$  is given by,

$$\gamma(r) = \frac{4}{3} \pi r_d^3 n(r)$$

where,  $n(r)$  is the number density of droplets at a particular  $r$  which refers to number of droplets per unit

volume. At steady state, we assume that the number density remains constant with respect to time at a particular distance from the nozzle.

$r_d$  is the droplet radius and is assumed to be uniform for all the droplets enclosed within the differential control volume.

#### Conservation of mass for the control volume:

Starting from Reynold's transport theorem for mass conservation we can write,

$$\frac{Dm_{sys}}{Dt} = \frac{\partial m_{CV}}{\partial t} + E_r$$

$$m_{sys} = \rho\gamma\Delta V$$

$$\therefore \frac{Dm_{sys}}{Dt} = \frac{d(\rho\frac{4}{3}\pi nr_d^3)}{dt} (\Omega r^2) dr$$

$$= \rho \left(\frac{4}{3}\pi nr_d^3\right) \frac{3}{r_d} \frac{dr_d}{dt} (\Omega r^2) dr$$

Here, number density of droplets is assumed to be constant with respect to time and only a function of the radial co-ordinate  $r$  at steady state. So, it is taken out of the time derivative. Let  $\mathbf{u}(r)$  be the velocity of the droplets at  $r$ .

Now, the velocity is given by,

$$\begin{aligned} u &= \frac{dr}{dt} \\ \therefore \frac{Dm_{sys}}{Dt} &= \rho\gamma(\Omega r^2) dr \left(u \frac{3}{r_d} \frac{dr_d}{dr}\right) \\ &= \rho\Omega(\gamma r^2 u) \frac{3dr_d}{r_d} \end{aligned} \quad (1)$$

And at steady state the mass of control volume doesn't change. Therefore:

$$\frac{\partial m_{CV}}{\partial t} = 0$$

The efflux  $E_r$  is given by,

$$E_r = \left(F_r + \frac{\partial F_r}{\partial r} dr\right) - F_r$$

where the mass flux  $F_r$  is given by,

$$F_r = \rho\gamma\Omega r^2 u$$

$$E_r = \frac{\partial(\rho\gamma\Omega r^2 u)}{\partial r} dr$$

Since at steady state, all the terms are functions of only the radial co-ordinate, this can be written as an absolute derivative:

$$E_r = \rho\Omega d(\gamma r^2 u) \quad (2)$$

Equating (1) and (2):

$$\rho\Omega(\gamma r^2 u) \frac{3dr_d}{r_d} = \rho\Omega d(\gamma r^2 u)$$

Integrating, we get

$$\ln \frac{(\gamma r^2 u)}{r_d^3} = c_1'$$

In the above equation,  $c_1'$  is a constant of integration.

Thus we obtain:

$$\frac{u\gamma r^2}{r_d^3} = c_1 \quad (3)$$

The value of  $c_1$  can be determined by initial conditions at breakup,

$$c_1 = \frac{u_0\gamma_0 R_0^2}{r_{d0}^3}$$

#### Conservation of momentum for the control volume:

This is applied to both the entrained gas and the fuel.

$$\frac{\partial}{\partial r} ((\rho_a(1-\gamma)v_a^2 r^2 + \rho\gamma u^2 r^2)) dr = 0$$

$$\Rightarrow (\rho_a(1-\gamma)v_a^2 r^2 + \rho\gamma u^2 r^2) = c_2 \quad (4)$$

Where the constant  $c_2$  can be found from initial conditions at breakup:

$$c_2 = (\rho_a(1-\gamma_0)v_{a0}^2 R_0^2 + \rho\gamma_0 u_0^2 R_0^2)$$

Here,  $v_{a0}$  is the velocity of the entrained ambient gas in the chamber at the breakup length and is a fraction ( $\frac{v_{a0}}{u_0} < 1$ ) of the fuel velocity at the breakup. Both numerical simulations and other models [9] have shown that the particular value of this fraction does not significantly affect the velocities of the entrained gas or the fuel at larger penetration lengths.

### Drag on a droplet:

The drag equation is formulated for a droplet and this determines the amount of momentum loss from the droplets in the liquid phase to the entrained gas.

$$\frac{1}{2} \rho_a C_D |(v_a - u)|(v_a - u) \pi r_d^2 = \frac{d}{dt} (\rho \frac{4}{3} \pi r_d^3 u) \quad (5)$$

Here, the drag coefficient ( $C_D$ ) is obtained from the relationship (Wallis (1969)) :

$$C_D = (24/Re)(1 + 0.5|Re|^{0.687})$$

for  $Re \leq 1000$  and  $C_D = 0.44$  for  $Re \geq 1000$ , where  $Re$  is the Reynolds number and is defined as:

$$Re = \frac{2r_d(u-v_a)\rho_a}{\mu_a}$$

The dynamic viscosity of the ambient gas ( $\mu_a$ ) is computed using the Lee-Gonzalez-Eakin correlation [9].

### Formulation for Evaporation:

Droplet evaporation is described using the  $D^2$  law:

$$r_d(t)^2 = r_{d0}^2 - kt$$

The differential form the above equation can be written as:

$$\frac{dr_d}{dr} = -\frac{k}{2ur_d} \quad (6)$$

The Ranz-Marshall correlation is employed to ascertain the convective evaporative constant as a function of the local Reynolds number and the Schmidt number. The convective evaporative constant is calculated to be about two orders of magnitude greater than the diffusive evaporative constant, and hence we can solely use the convective constant for describing evaporation.

The evaporative constant depends on multiple factors such as diffusivity in the medium, saturation pressure of the fuel, the ambient pressure and temperature and also on the Reynolds and Schmidt numbers. The Reynolds number is as defined earlier and the Schmidt number is defined as:

$$Sc = -\frac{\mu_a}{\rho_a D},$$

where  $D$  represents the molecular diffusivity of the fuel in the ambient gas in chamber.

Now, equations (3), (4), (5) and (6) are solved numerically to obtain the velocity at any point in the spray ( $u(r)$ ) and the volume fraction ( $\gamma(r)$ ) in region 1 of the spray.

### c. Accommodating jump conditions at the tip of the spray:

Consideration of the deformation of the spray near the front edge (region 2), is required to successfully predict the penetration. As stated earlier it is observed frequently that sprays in highly pressurized surroundings develop vortex like ring structures. These mushroom shaped plumes suggest that there is momentum accumulation at the tip of the spray, caused due to excessive drag.

The fuel volume fraction ( $\gamma$ ) goes to zero suddenly at the tip due to momentum accumulation and compression of the spray. The tip velocity ( $U_t$ ) is thus significantly lower than the nominal velocity of the droplets of the spray. If we consider a moving control volume, moving at the tip velocity, at the tip of the spray enclosing part of the tip and just outside the tip and write the momentum conservation equation, we obtain:

$$(\rho\gamma + \rho_a(1 - \gamma))(u - U_t)^2 = \frac{\rho_a U_t^2}{2}$$

where the term on the left is the momentum flux of the spray entering the control volume and the term on the right represents stagnation pressure of the air in front of the spray. Rearranging we obtain,

$$U_t = u * \left(1 + \sqrt{\frac{\rho_a}{2(\rho_a + \Delta\rho\gamma)}}\right)^{-1} \quad (7)$$

Now, the differential equation for temporal tip velocity is given by:

$$\frac{dR_t}{dt} = U_t \quad (8)$$

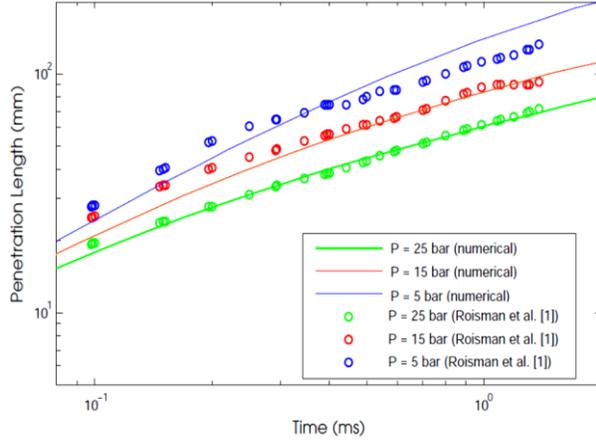
here,  $R_t$  represents the penetration length of the spray tip.

Now, the solutions for  $u$  and  $\gamma$  from region-1 of the spray are used in equation (7) and subsequently the equation (8) is integrated to obtain the penetration length of the spray as a function of time.

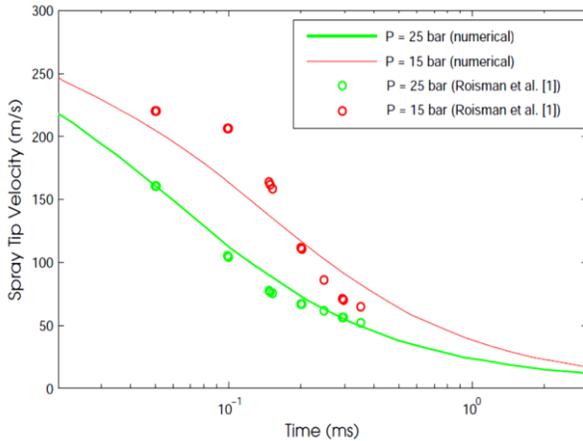
## 4. Base Model Validation

The base model which is taken from Roisman et al. [1] has been validated against the data reported by the same authors. This is done to ensure the proper implementation of the model. The different ambient pressures change the ambient air density and thus also affect the breakup of the spray. Hence, the droplet radius at breakup ( $r_{d0}$ ) is employed as a tunable constant. The solutions thus obtained from the numerical solution

setting the evaporative constant ( $k$ ) as zero (non-evaporative spray) compare reasonably well with the results. This can be seen from Fig. 2 which shows variation of spray penetration with time and Fig. 3 which shows the variation of tip velocity with time. The model thus accurately portrays the decrease in the penetration length and increase in tip velocity with the increase in the ambient pressure.

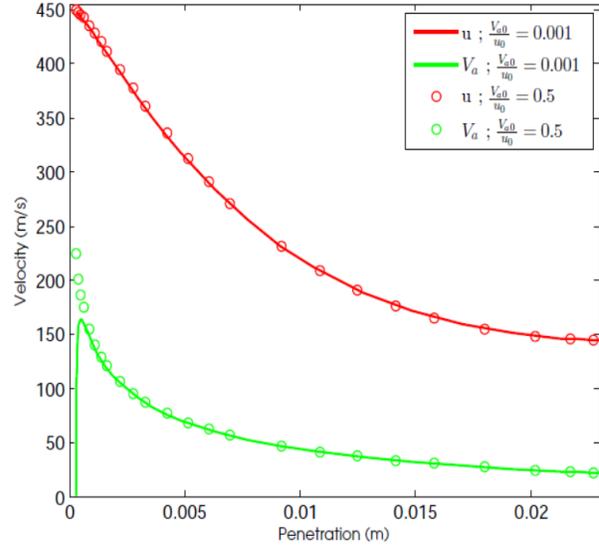


**Figure 2.** Plot comparing the penetration length of a non-evaporating diesel spray as evaluated by the numerical model (solid lines) with results (‘o’) from Roisman et al. [1].



**Figure 3.** Plot comparing the Spray tip velocity of a non-evaporating diesel spray as evaluated by the numerical model (solid lines) with experimental results (‘o’) from Roisman et al. [1].

The velocity of gas entrained in the spray at breakup is  $v_{a0}$  and since the momentum of the gas is transferred from the fuel droplets,  $v_{a0}$  will be a fraction of  $u_0$ . This fraction is the initial slip factor ( $\frac{v_{a0}}{u_0}$ ). It has been shown from simulations (Fig.4) that the velocities of the droplet ( $u$ ) and entrained gas ( $v_a$ ) further downstream are independent of the initial slip factor confirming this result as established in other models ([4]).



**Figure 4.** Plot comparing the droplet and entrained gas velocity distribution of a spray with initial slip factor  $\frac{v_{a0}}{u_0}$  set as 0.001 (solid line) and 0.5 (‘o’)

## 5. Results and discussion

In order to analyze the effect of evaporation on the penetration length of evaporating sprays, simulations involving hexane sprays have been designed as follows. Since breakup parameters may depend on the ambient pressure, gas density and temperature, an analysis decoupling the effects of evaporation from those of change in breakup parameters and ambient gas density has been opted for. This has been done by choosing a mixture of gases in the chamber in each subsequent case, keeping the ambient pressure, temperature and breakup parameters constant and only changing the mole fractions of the constituents of the ambient gas in the chamber so as to change the effective binary diffusivity of the fuel in the medium and thus solely change the evaporative constant.

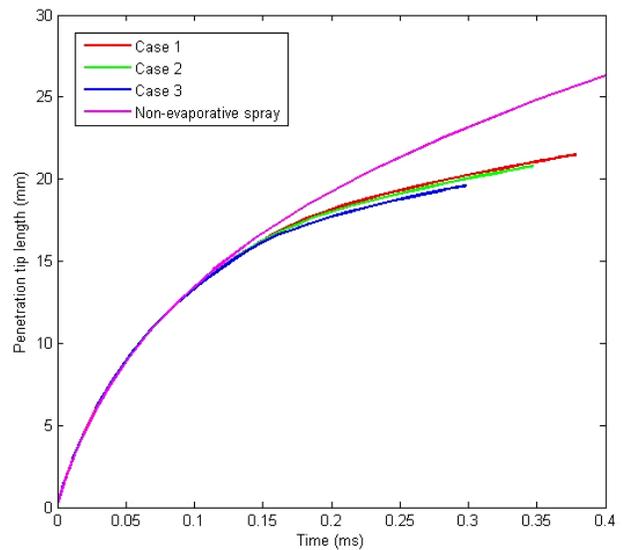
The results of the simulations are plotted in Fig.5 with the corresponding ambient gas constitution provided in Table 2. The effective binary diffusivity in each case has been computed as the weighted average of the individual binary diffusivities of hexane in each of the constituent ambient gases, weighted by their respective mole fractions in the chamber. The individual binary diffusivities have been evaluated employing the Fuller, Schettler and Giddings correlation [10]. It can be seen from Fig.5 that, as the effective binary diffusivity and hence the evaporative constant featuring in the  $D^2$  law increases with each subsequent case (1, 2 and 3), the spray droplet diameter decreases faster. Hence, at any given time the droplet diameters of the spray in Case 1 are greater than those in Case 2 and the ones in Case 2 greater than Case 3. Thus, the spray in Case 3 terminates the fastest, followed by the one in Case 2 and then the one in Case 1. The tip penetration plots in Fig.5 terminate upon the complete evaporation of the droplets.

It can also be observed that the penetration length of more evaporative sprays at later instances is lesser than that of a less evaporative spray. This can be attributed to the fact that less evaporative sprays have larger droplets than the more evaporative sprays at any instant. The greater inertia of the larger droplets in this scenario overcomes the larger drag since inertia scales as  $r_d^3$  and drag force scales as  $r_d^2$ .

Essentially, evaporating spray penetration shows significant deviation from non-evaporating spray penetration according to this model.

Case no.	$X_{He}$	$X_{CO_2}$	$X_{N_2}$	$D_{ab}^* \cdot 10^{-6} (m^2/s)$
1	0.4	0.1	0.5	1.228
2	0.4667	0.2	0.3333	1.318
3	0.6	0.4	0	1.496

**Table 2.** Mole fractions of the different components of the ambient gas and its effective diffusivity in the chamber in each case.



**Figure 5.** Plot comparing the penetration length as a function of time for evaporating hexane sprays in different ambient gases. The composition of ambient gases in each case is given in Table 2.

## 6. Conclusion

It can be understood from the above model that by incorporating the effects of droplet evaporation in spray penetration, we can observe deviation from the penetration length predicted for a non-evaporative spray. Though the analysis has been performed taking an azimuthally invariant conical spray, the observed deviation should also hold true for sprays with more realistic velocity and droplet size distributions. In addition, the change in penetration due to change in evaporation in different media can also be effectively analyzed with this model.

## References

- [1] Roisman, I. V., Lucio Araneo, and C. Tropea. "Effect of ambient pressure on penetration of a diesel spray." *International journal of multiphase flow* 33.8 (2007): 904-920.
- [2] Wan, Yuepeng, and Norbert Peters. "Scaling of spray penetration with evaporation." *Atomization and Sprays* 9.2 (1999).
- [3] Sazhin, S. S., G. Feng, and M. R. Heikal. "A model for fuel spray penetration." *Fuel* 80.15 (2001): 2171-2180.
- [4] Ghosh, S., and J. C. R. Hunt. "Induced air velocity within droplet driven sprays." *Proceedings of the*

*Royal Society of London A: Mathematical, Physical and Engineering Sciences*. Vol. 444. No. 1920. The Royal Society, 1994.

- [5] Turns, Stephen R. - An Introduction to Combustion - Concepts and Applications (2ed, McGraw-Hill).
- [6] Stauffer, D., 1979. Scaling theory of percolation clusters. *Phys. Rep.* 54, 1–74.
- [7] Stauffer, D., 1985. Introduction to Percolation Theory. Taylor & Francis, London.
- [8] Yarin, A.L., 1993. Free Liquid Jets and Films: Hydrodynamics and Rheology. Longman & Wiley, New York.
- [9] Lee, Anthony L., Mario H. Gonzalez, and Bertram E. Eakin. "The viscosity of natural gases." *Journal of Petroleum Technology* 18.08 (1966): 997-1.
- [10] Fuller, Edward N., Paul D. Schettler, and J. Calvin Giddings. "New method for prediction of binary gas-phase diffusion coefficients." *Industrial & Engineering Chemistry* 58.5 (1966): 18-27.

