Sooting premixed C_2H_2 counter flow flames:

Comparison of Measurements and Model Calculations

Elke Goos, Peter Frank

Institute of Combustion Technology, German Aerospace Center (DLR), Pfaffenwaldring 38-40, D-70569 Stuttgart, Germany

Beate Jungfleisch, Rainer Suntz, Henning Bockhorn

Institute for Chemical Technology, University of Karlsruhe (TH), Kaiserstrasse 12, D-76131 Karlsruhe, Germany

Why modeling soot formation ?

Combustion devices: e.g. aircrafts, cars, gas turbines,…

Emissions: e.g. NO_x, PAH, Soot, ...

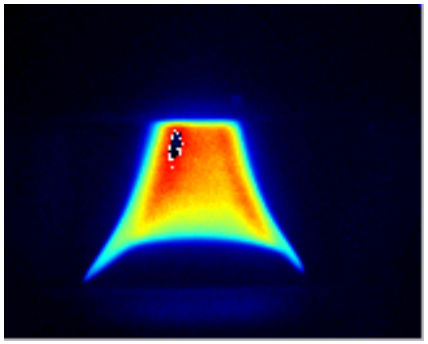
Regulations for amount of pollutants
e.g. EURO III, EURO IV

Reduction of emissions at sources desirable

Detailed understanding of formation process and formation conditions

Why not modeling a technical combustion process ?

Flame:

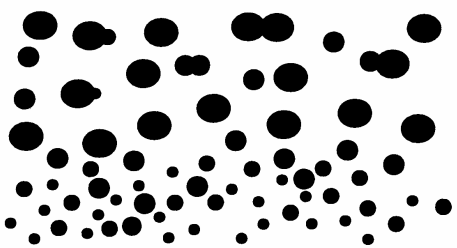


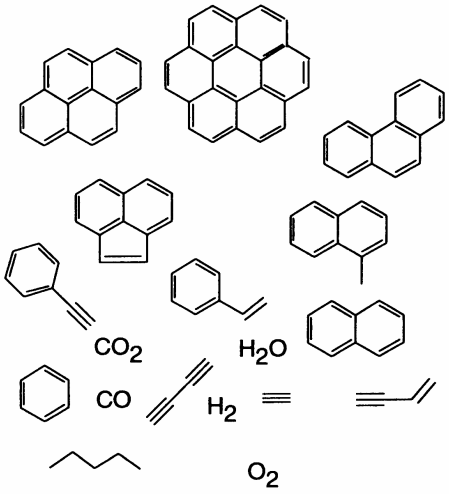
Averaged soot distribution
C_3H_6 flame, 1 bar, f = 2.15

Necessary information:

Fluid dynamic
+
Reaction kinetics

Soot model:





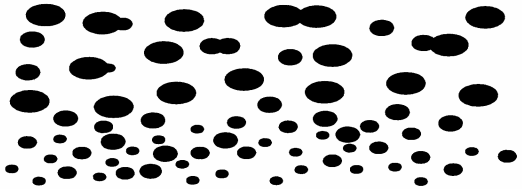
Experimental validation: **Dependent on pressure, fuel, equivalence ratio**

„Soot Formation in Combustion, Mechanisms and Models", Ed. H. Bockhorn, Springer Series in Chemical Physics, Heidelberg, 59, 1994

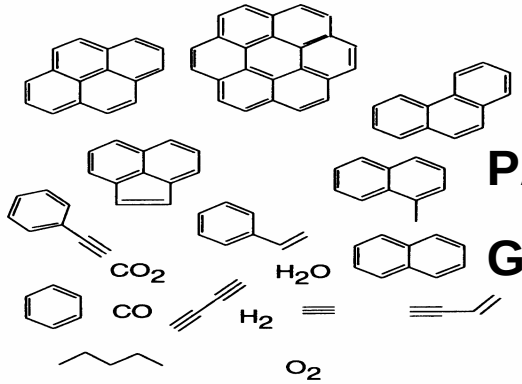
Soot formation and decomposition

time

Surface Growth, Coagulation
Surface Oxidation



Particle Inception (Coagulation)



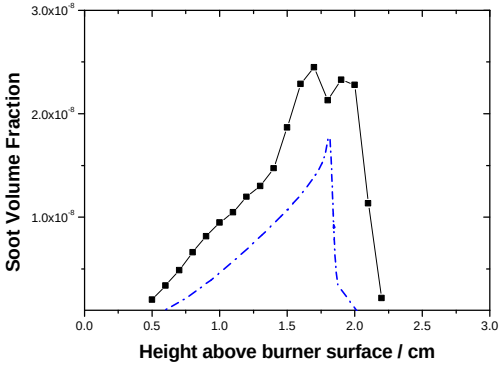
PAH

Growth

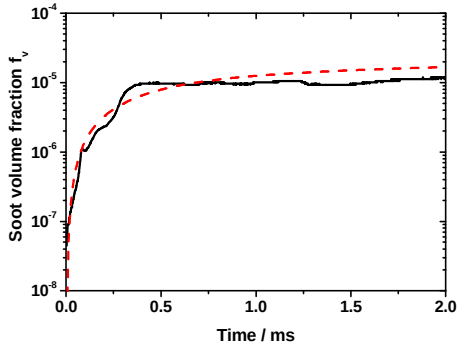
Detailed Gas Phase Chemistry (Fuel specific)

Original picture from „Soot Formation in Combustion, Mechanisms and Models", Ed. H. Bockhorn, Springer Series in Chemical Physics, Heidelberg, 59, 1994

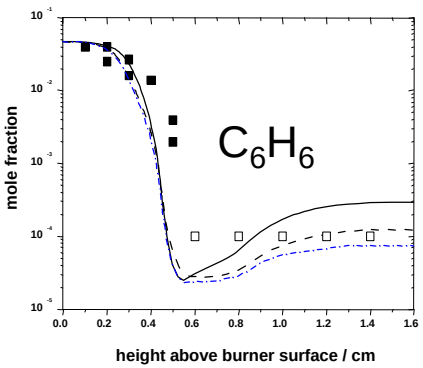
Counter flow
C_2H_2 Diffusion flame:

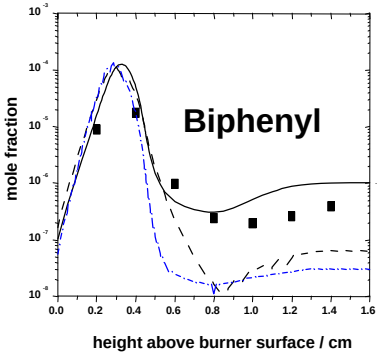


Shock tube experiment:
1-methylnaphthalene/argon
p = 16 bar, T = 1700 K



Benzene air flame: 1 bar C/O=0.72:





Soot growth and soot oxidation

Surface radical production: $C_{soot}\text{-}H + H = C_{soot}^{\cdot} + H_2$

Recombination of radicals: $C_{soot}^{\cdot} + H = C_{soot}\text{-}H$

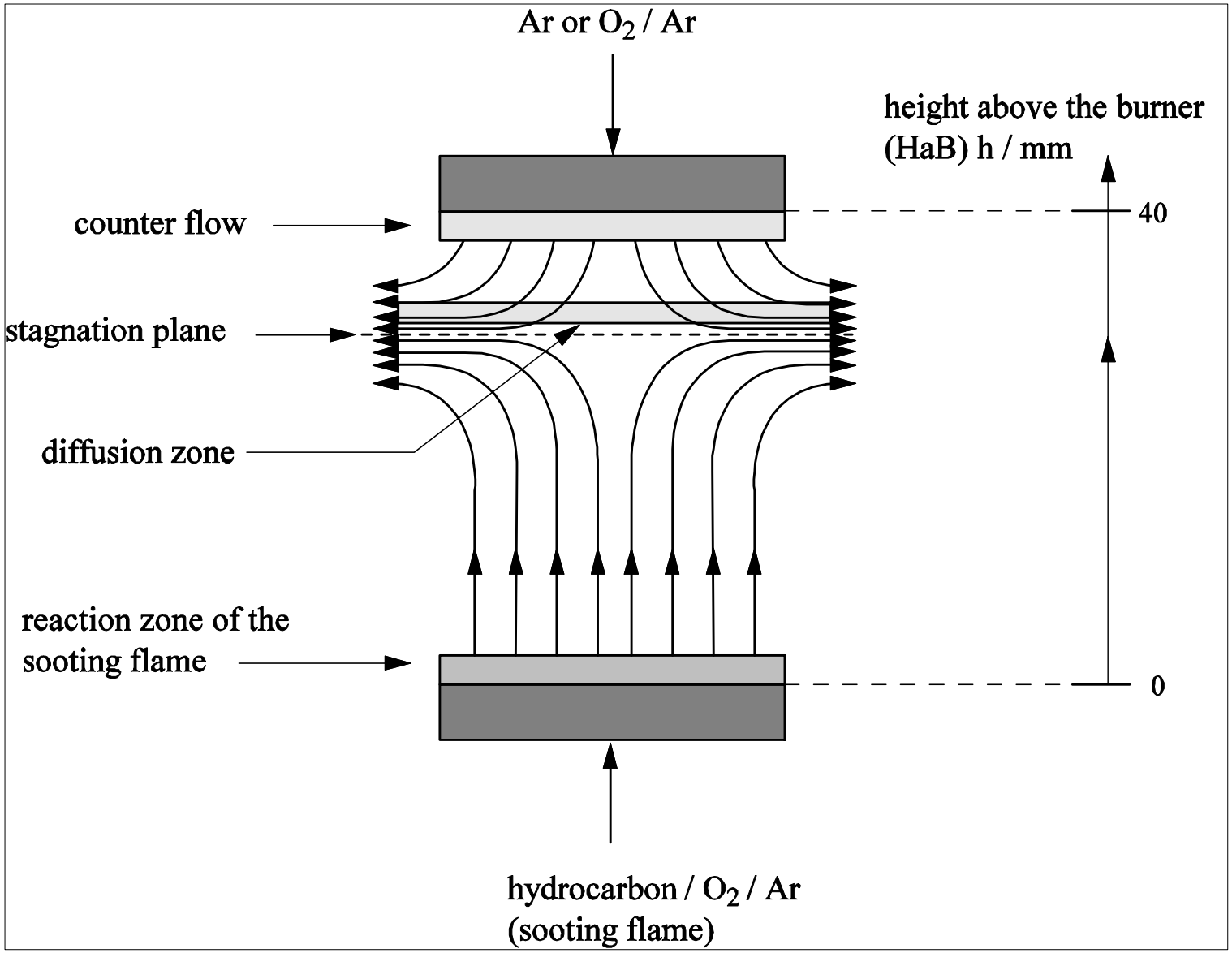
Soot growth: $C_{soot}^{\cdot} + C_2H_2 = C_{soot+C2}\text{-}H + H$

Oxidation of the soot particles: $C_{soot}\text{-}H + OH = \text{products}$

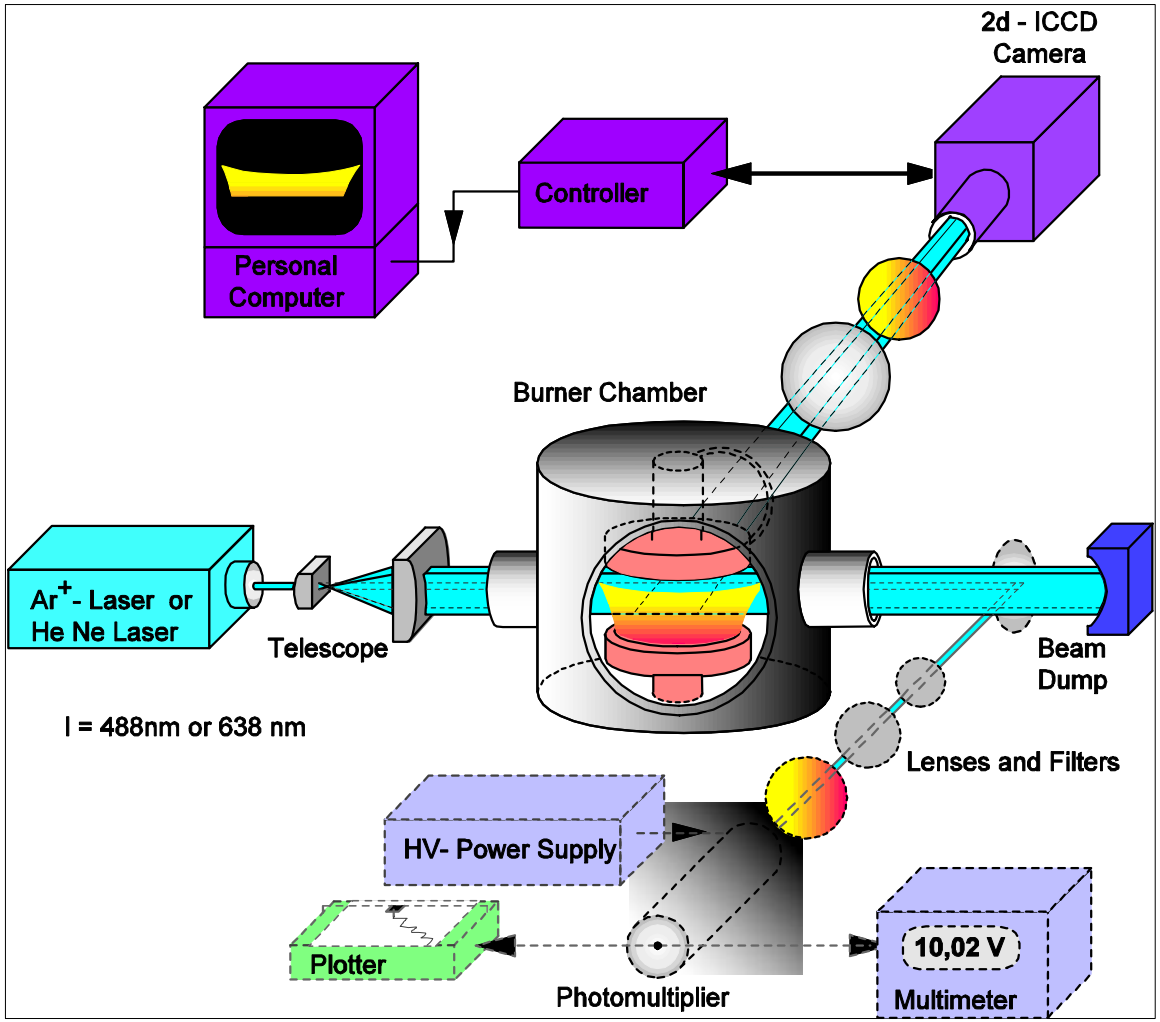
$C_{soot}^{\cdot} + O_2 = \text{products}$

$$R(T) = k_{perSite}\,[Species_{Gasphase}]\; a\;\; c_{Sootradical}\; N_i^{soot}$$

Low pressure premixed flat C_2H_2 flames in a counter flow configuration



Experimental setup :
Rayleigh scattering / extinction technique

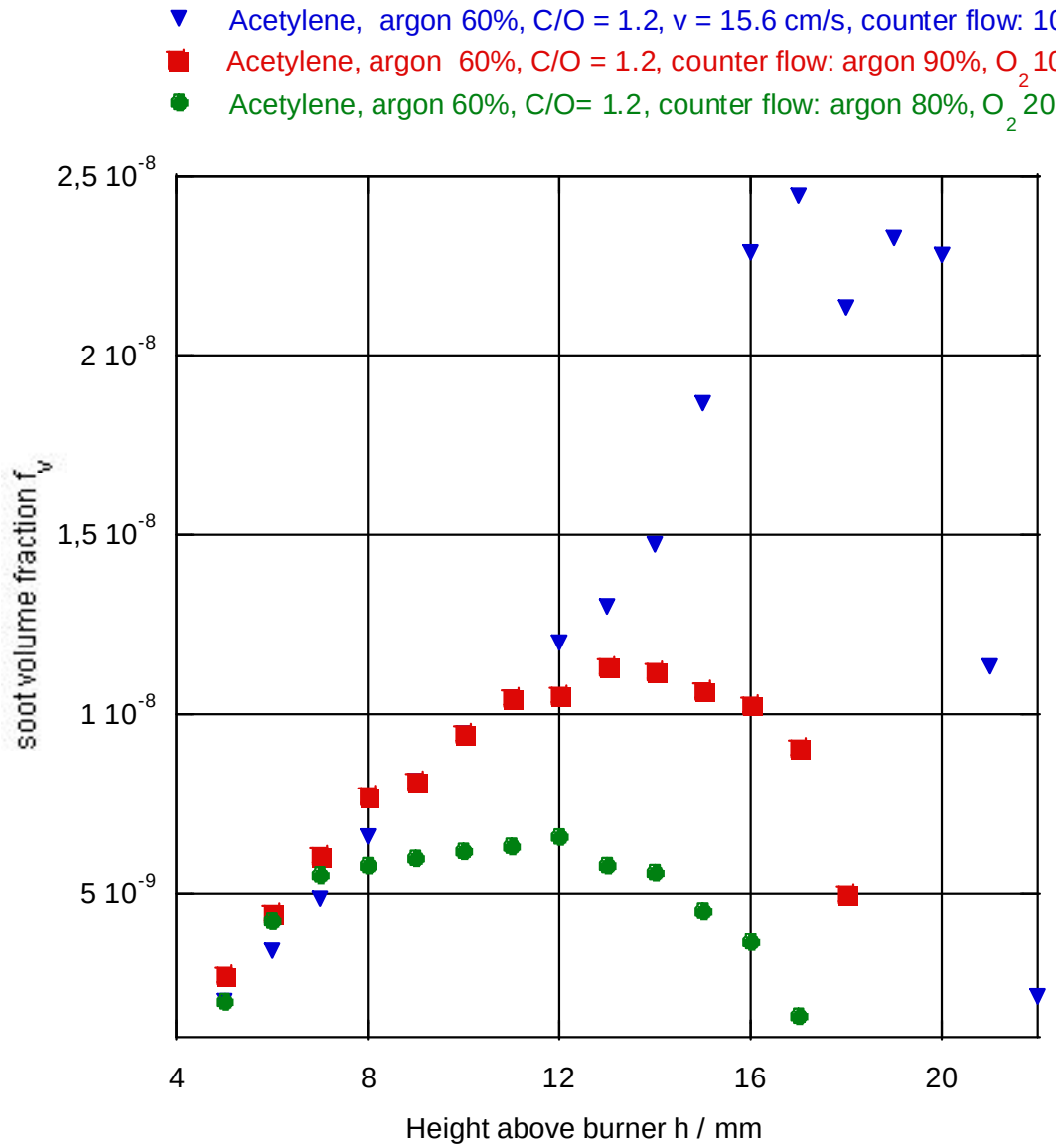


- Signals are induced by a Ar^{+} or a He-Ne Laser
- Extinction is detected by a photomultiplier
- Scattered light is detected by a ICCD camera

Premixed C_2H_2 flames in counter flow configuration

	Flame 1 (F1)	Flame 2 (F2)	Flame 3 (F3)
Counter flow side:	100 % Ar	90 % Ar 10 % O_2	80 % Ar 20 % O_2
Flow side:	C_2H_2, O_2, Ar-flame C/O = 1.2 , 60 % Ar 90 mbar		

Experimental results: soot volume fractions

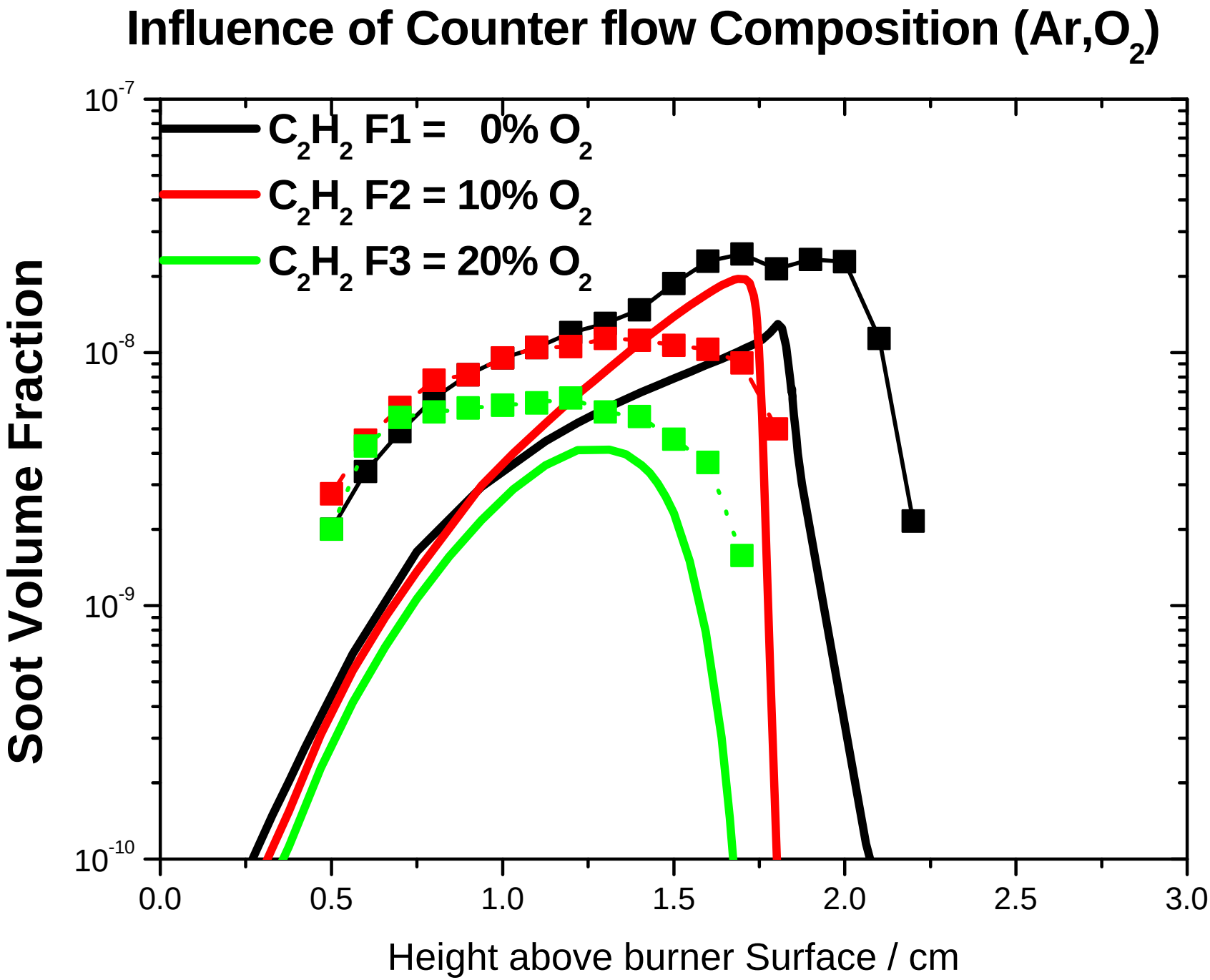


- Argon counter flow:
Steep increase of f_V at 15 mm HaB

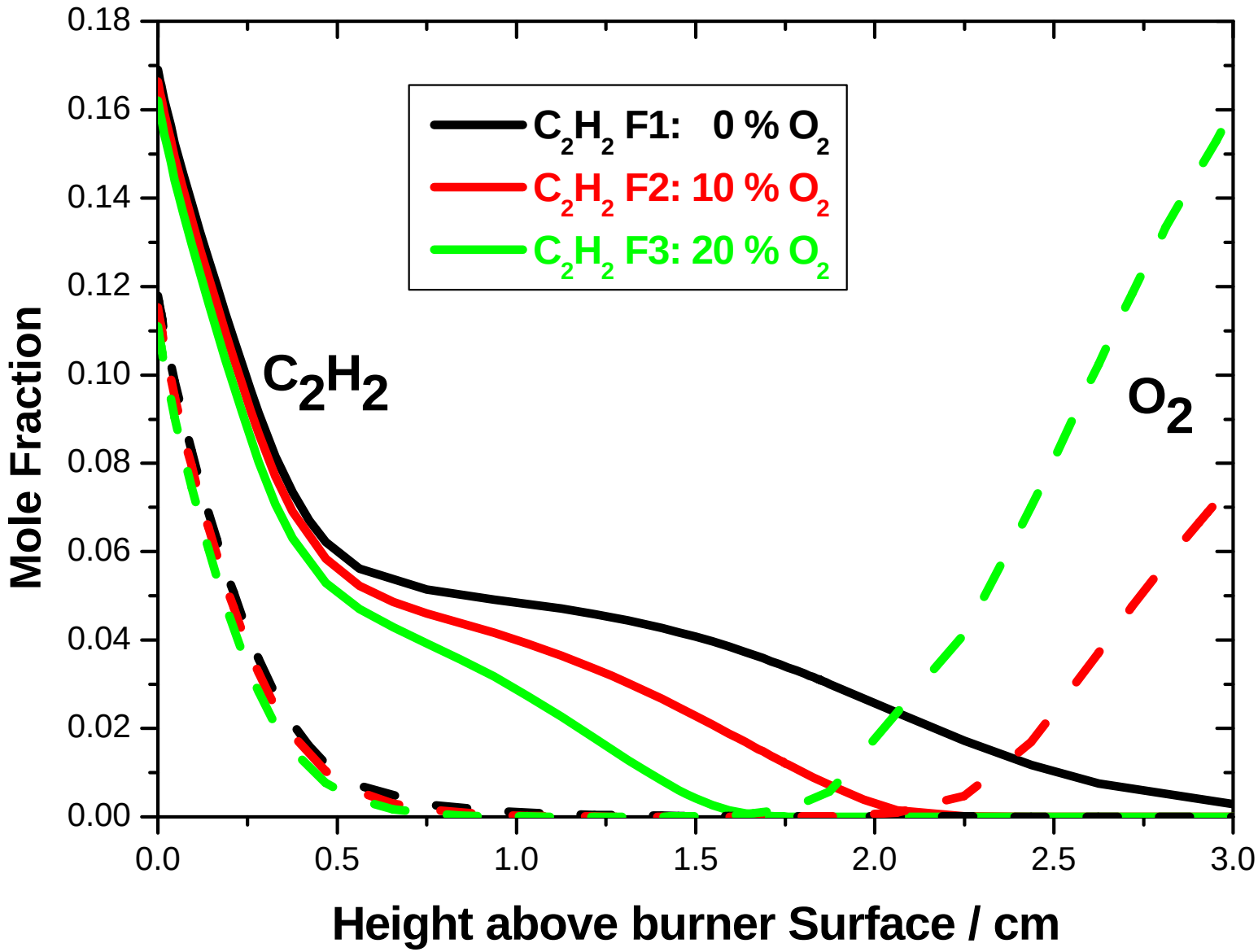
-Addition of O_2 in counter flow:

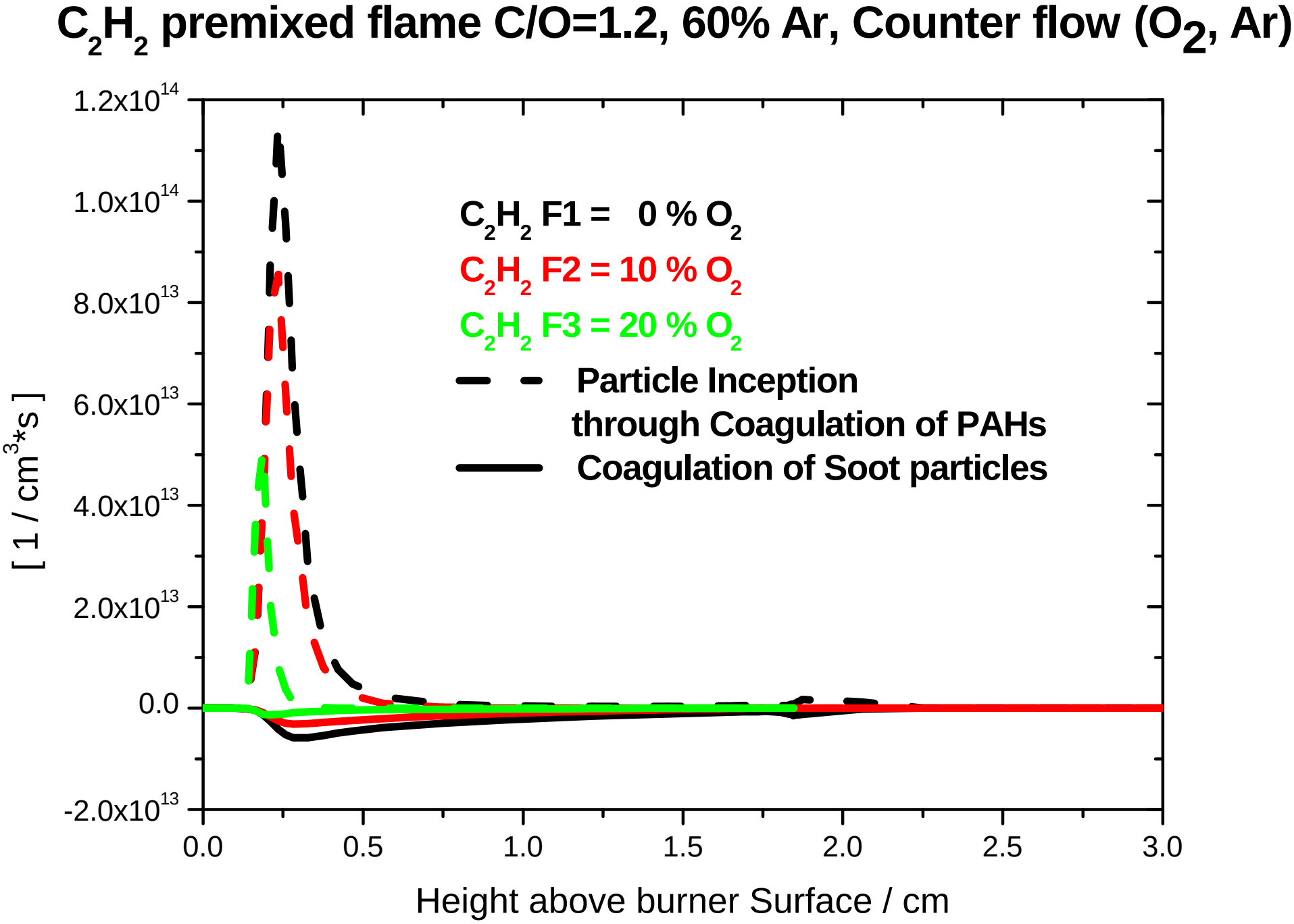
- Decrease of the maximum of f_V
- Shift of the maximum of f_V to lower HaB

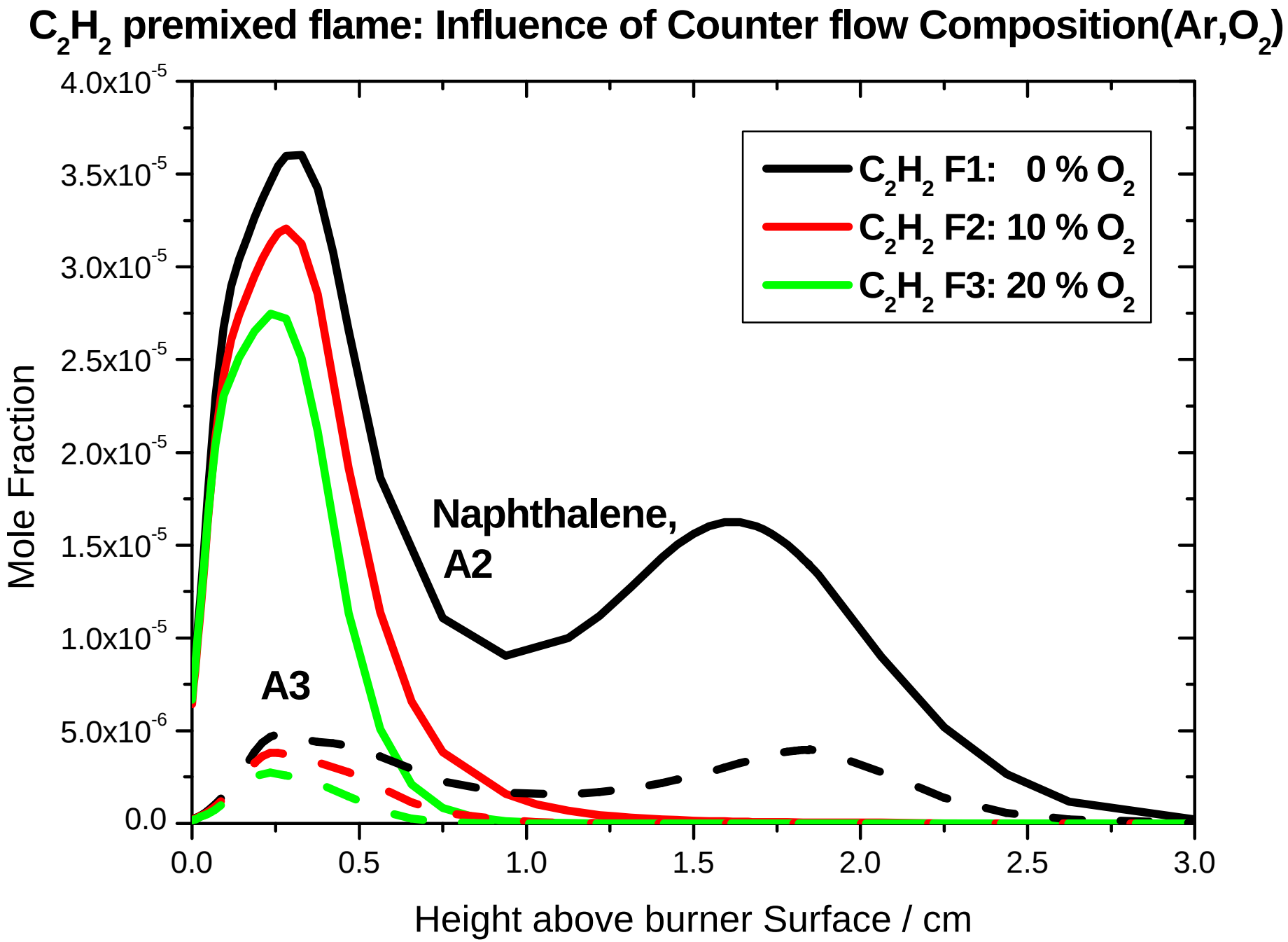
= displacement of the stagnation plane

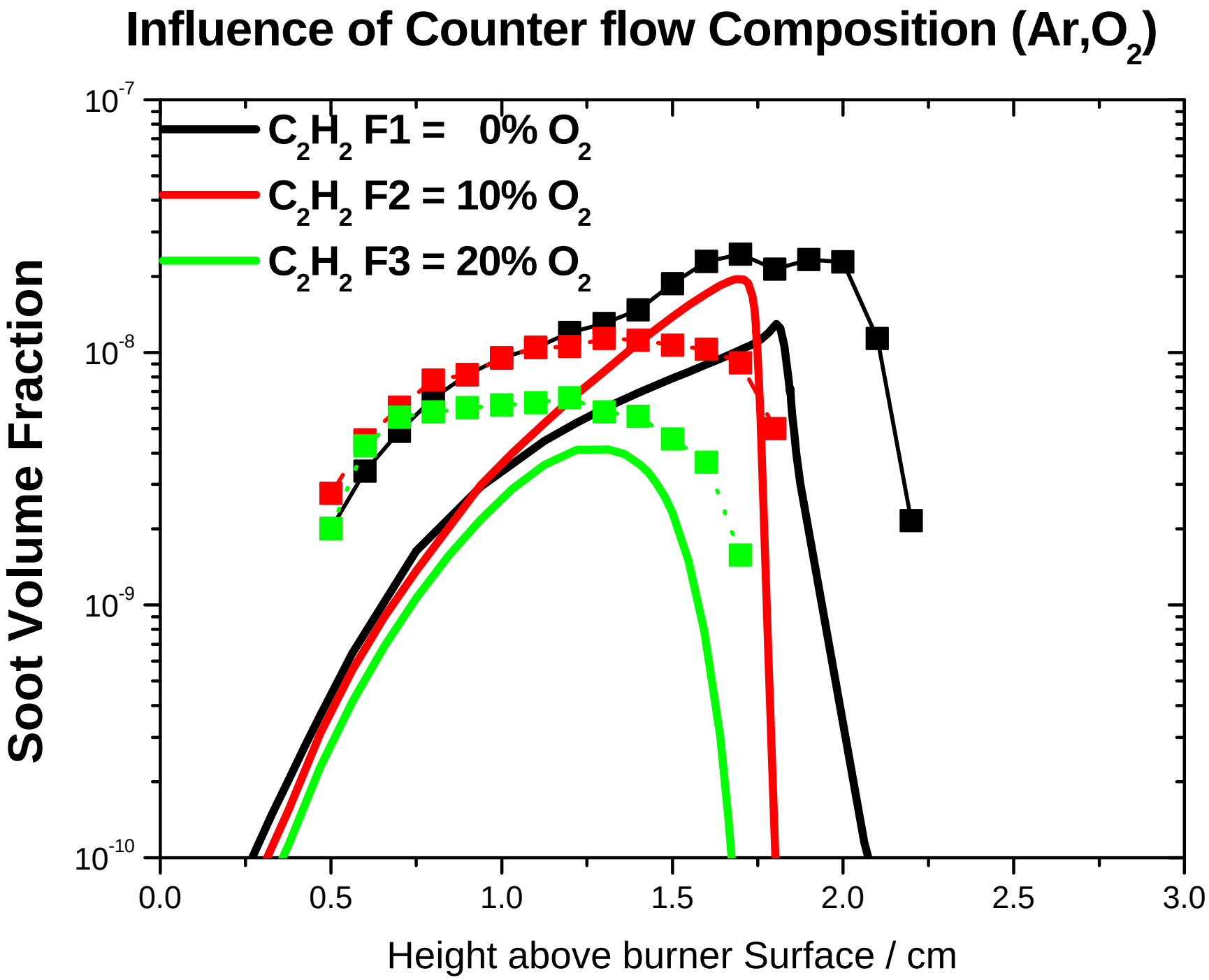

Influence of Counter flow Composition (Ar,O2)
C2H2 F1 = 0% O2
C2H2 F2 = 10% O2
C2H2 F3 = 20% O2
Soot Volume Fraction
10-7
10-8
10-9
10-10
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Height above burner Surface / cm

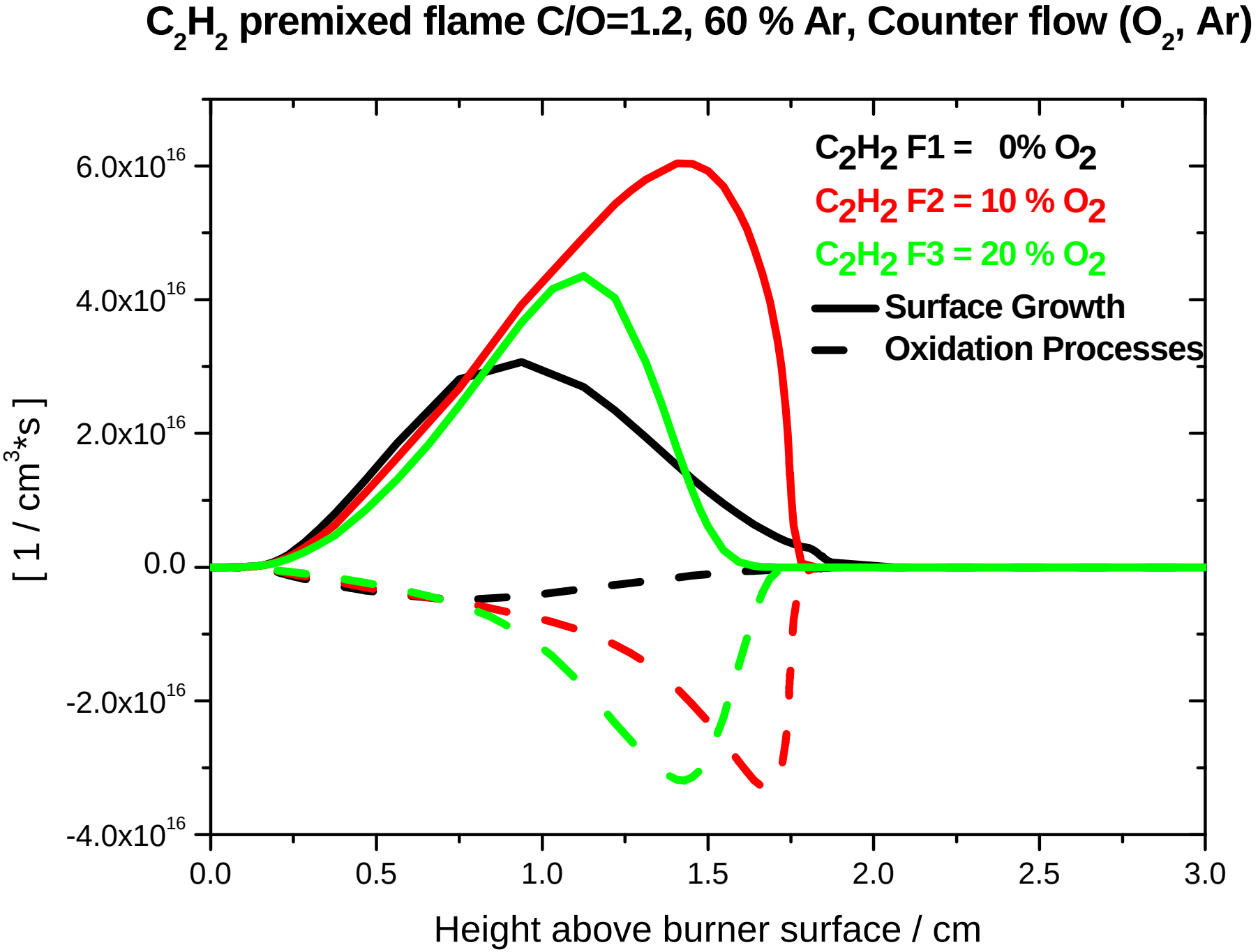
C_2H_2 premixed flame: Influence of Counter flow Composition (Ar,O_2)

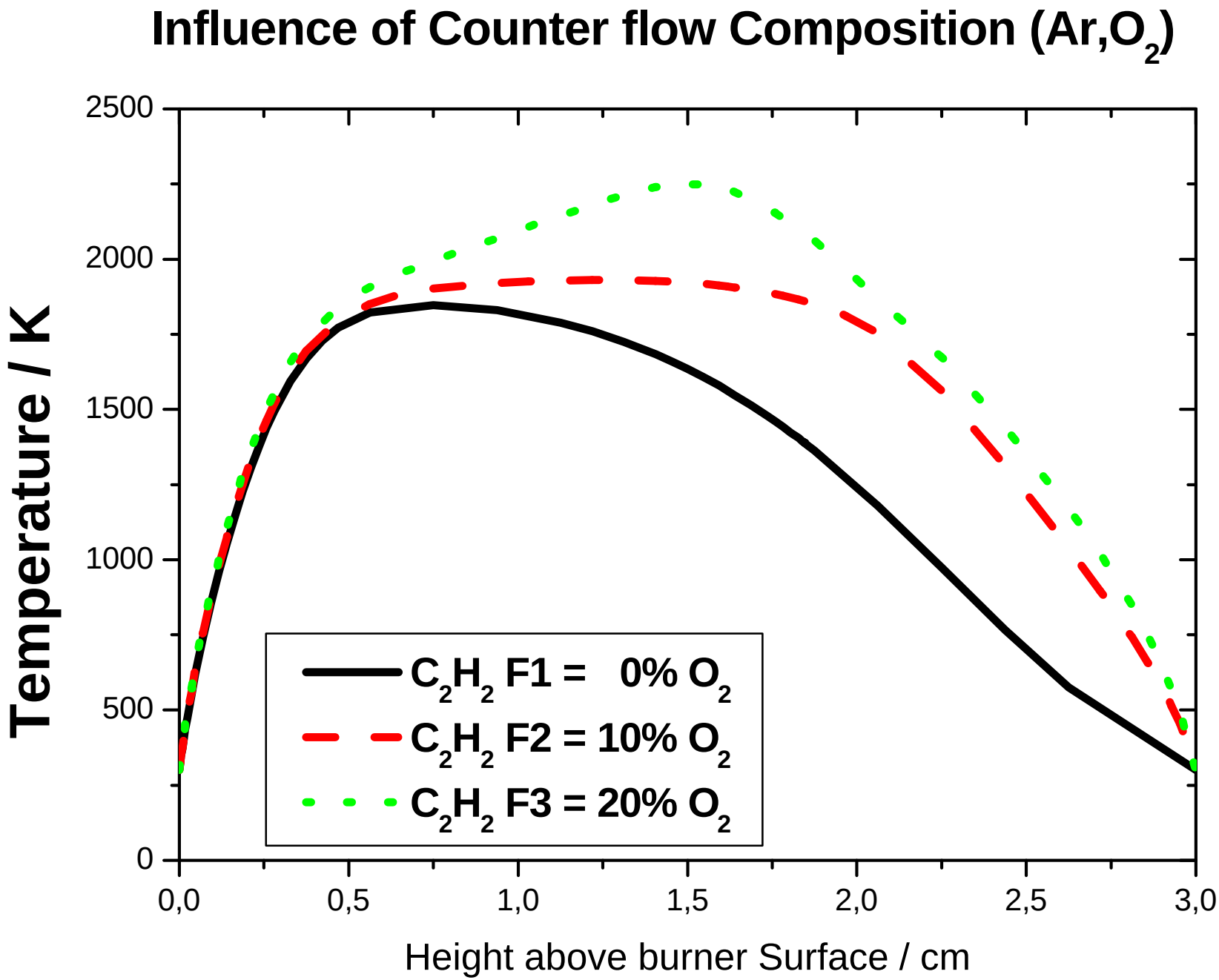



C2H2 premixed flame C/O=1.2, 60% Ar, Counter flow (O2, Ar)
1.2x10^14
1.0x10^14
8.0x10^13
6.0x10^13
4.0x10^13
2.0x10^13
0.0
-2.0x10^13
[1 / cm^3*s]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Height above burner Surface / cm
C2H2 F1 = 0 % O2
C2H2 F2 = 10 % O2
C2H2 F3 = 20 % O2
Particle Inception
through Coagulation of PAHs
Coagulation of Soot particles


C2H2 premixed flame: Influence of Counter flow Composition(Ar,O2)
4.0x10-5
3.5x10-5
3.0x10-5
2.5x10-5
2.0x10-5
1.5x10-5
1.0x10-5
5.0x10-6
0.0
Mole Fraction
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Height above burner Surface / cm
C2H2 F1: 0 % O2
C2H2 F2: 10 % O2
C2H2 F3: 20 % O2
Naphthalene,
A2
A3


Influence of Counter flow Composition (Ar,O2)
C2H2 F1 = 0% O2
C2H2 F2 = 10% O2
C2H2 F3 = 20% O2
Soot Volume Fraction
10-7
10-8
10-9
10-10
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Height above burner Surface / cm


C2H2 premixed flame C/O=1.2, 60 % Ar, Counter flow (O2, Ar)
C2H2 F1 = 0% O2
C2H2 F2 = 10 % O2
C2H2 F3 = 20 % O2
Surface Growth
Oxidation Processes
6.0x10^16
4.0x10^16
2.0x10^16
0.0
-2.0x10^16
-4.0x10^16
[1 / cm^3*s]
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Height above burner surface / cm


Influence of Counter flow Composition (Ar,O2)
Temperature / K
2500
2000
1500
1000
500
0
0,0
0,5
1,0
1,5
2,0
2,5
3,0
Height above burner Surface / cm
C2H2 F1 = 0% O2
C2H2 F2 = 10% O2
C2H2 F3 = 20% O2

Summary

Investigations at sooting premixed C_2H_2 flames with different counter flow conditions:

- **Measurements of soot volume fractions, temperature**
- **Calculation of measured conditions**
- **Comparison of results**

=> Model calculations explain experimental trends

=> Calculate influence of the gas phase model, the temperature profile on the soot formation

Separation of soot inception process from soot growth and soot decomposition processes possible

=> Soot model will be improved