An Updated Reaction Model for the High-Temperature Pyrolysis and Oxidation of Acetaldehyde

R. Mével*[,a,b], K. Chatelain[c], G. Blanquart[d], J.E. Shepherd[e]

[a] *Center for Combustion Energy, Tsinghua University, Beijing 100084, China*
[b] *Department of Automotive Engineering, Tsinghua University, Beijing 100084, China*
[c] *ENSTA-ParisTech, Paris-Saclay University, Palaiseau, France*
[d] *Mechanical Engineering Department, California Institute of Technology, Pasadena, CA, USA*
[e] *Graduate Aerospace Laboratories, California Institute of Technology, Pasadena, CA, USA*

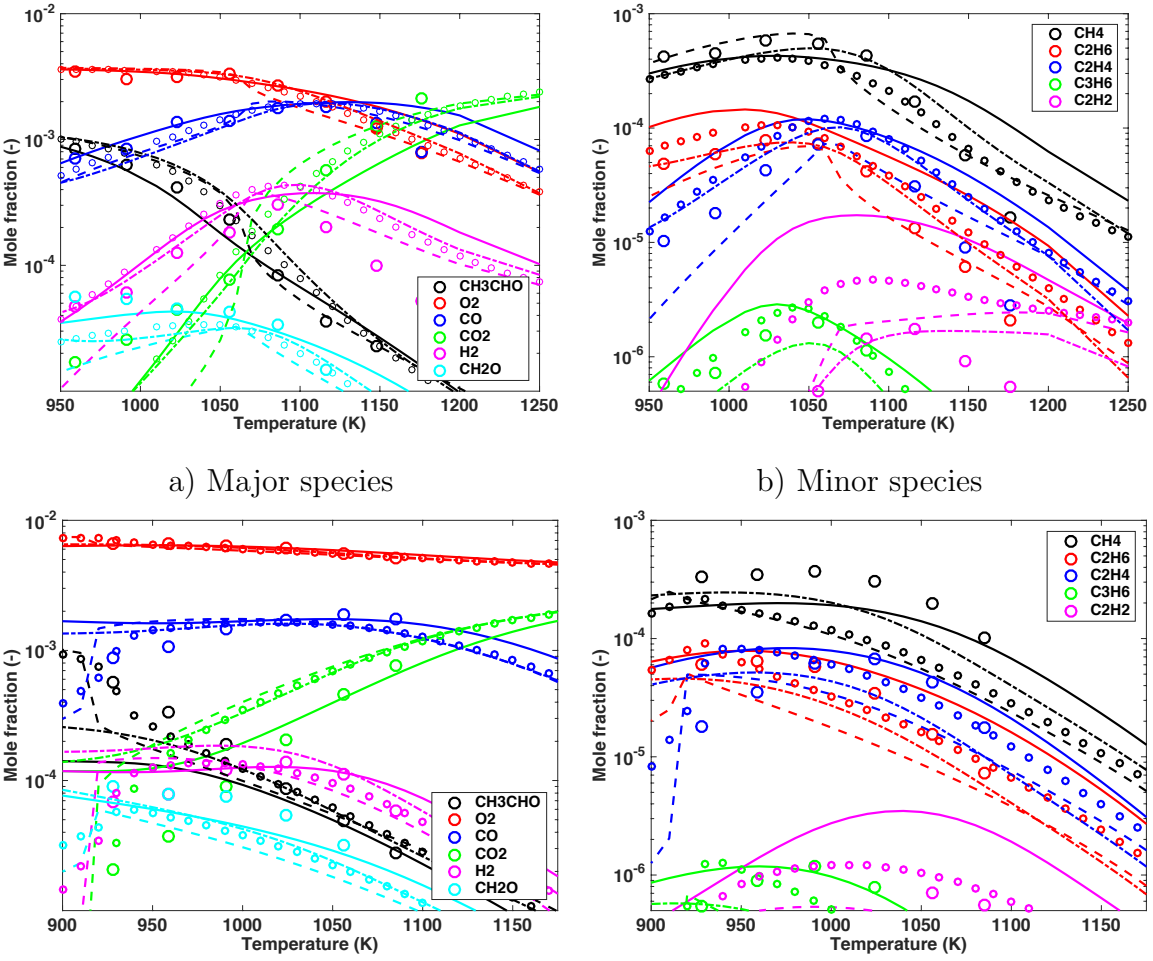
Additional modeling results

This supplemental material presents additional modeling results for data obtained with experimental facilities other than shock tubes. For these calculations, only the C_1-C_3 part of the Aramco 2.0 and JetSurf models have been used. In addition, the "PLOG_replace" routine from C^3 NUI Galway has been employed to generate pressure specific reaction rates for the PSR calculations performed with the Aramco 2.0. For the new model proposed in the present study, the flame speed and flame structure calculations have been performed without the sub-mechanism for vinyl alcohol and nitrogen has been considered as non-reactive. Solid, dashed-dotted, dotted, and dashed lines are used for the present model's, Aramco's, CaltechMech's, and JetSurf's results, respectively.

*Corresponding author: mevel@mail.tsinghua.edu.cn

Jet-stirred reactor

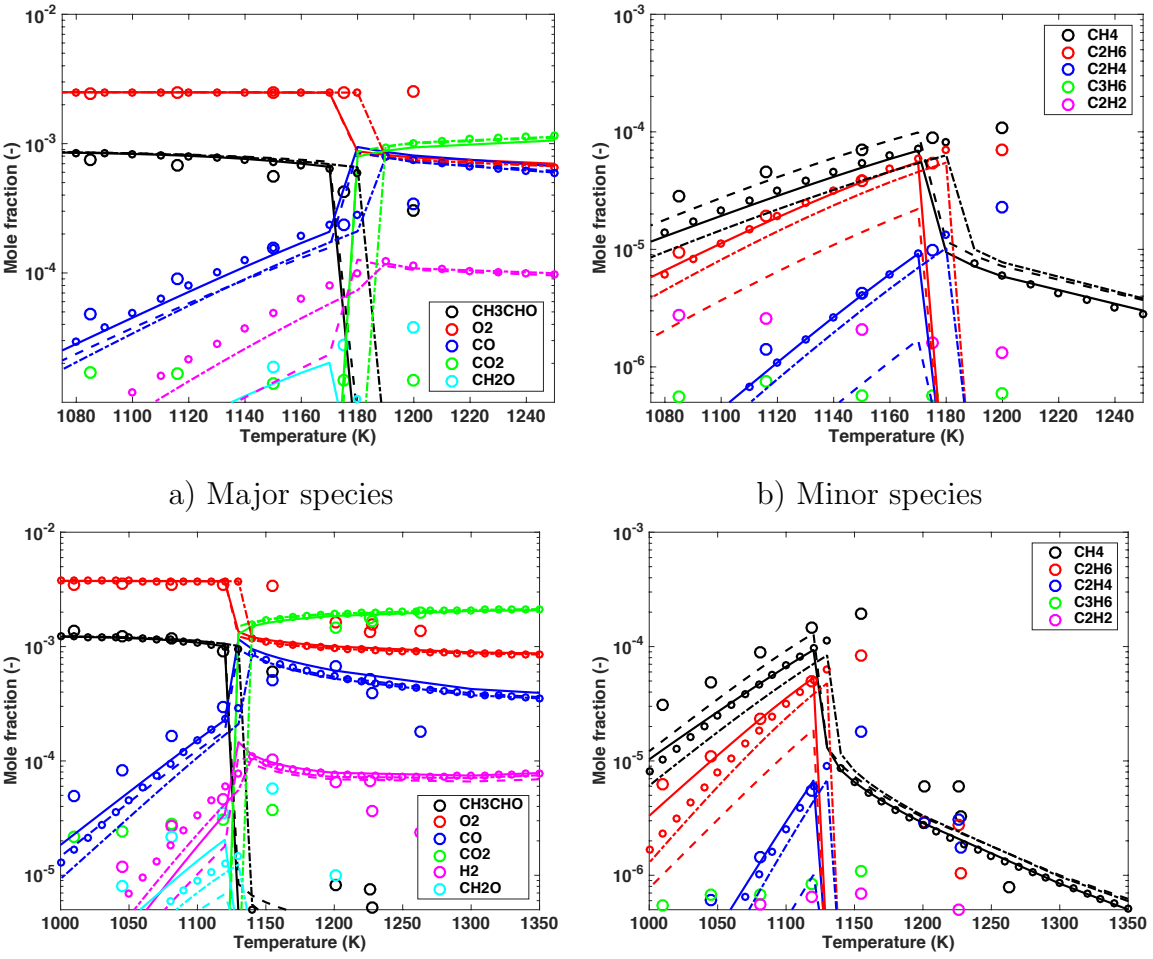
Jet-stirred reactor data from Dagaut et al. study [1] have been modeled using the PSR code from Chemkin II package. Figure 1 shows a comparison between the experimental data and the predictions of the four models previously used for the ST modeling study.



a) Major species b) Minor species

c) Major species d) Minor species

Figure 1: Comparison between the experimental [1] and the predicted species profiles for acetaldehyde-oxygen-nitrogen mixtures in a jet stirred reactor. Conditions in a) and b): Φ=1; X_{N2}=0.99475; P=1013 kPa; residence time=0.8 s. Conditions in c) and d): Φ=0.43; X_{N2}=0.9922; P=1013 kPa; residence time=0.8 s.



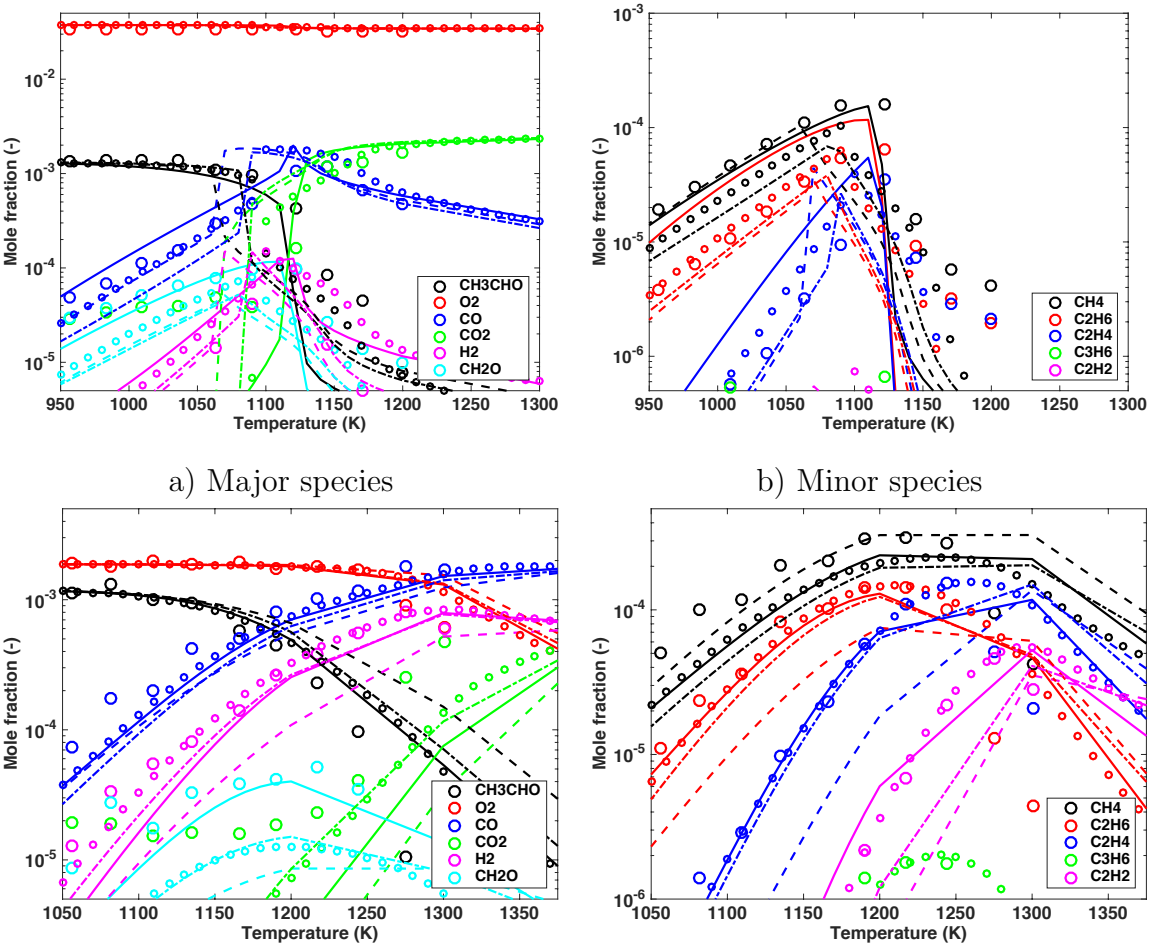
a) Major species

b) Minor species

c) Major species

d) Minor species

Figure 2: Comparison between the experimental [1] and the predicted species profiles for acetaldehyde-oxygen-nitrogen mixtures in a jet stirred reactor. Conditions in a) and b): Φ=0.88; X_{N2}=0.99662; P=101 kPa; residence time=0.04 s. Conditions in c) and d): Φ=0.83; X_{N2}=0.99501; P=101 kPa; residence time=0.08 s.



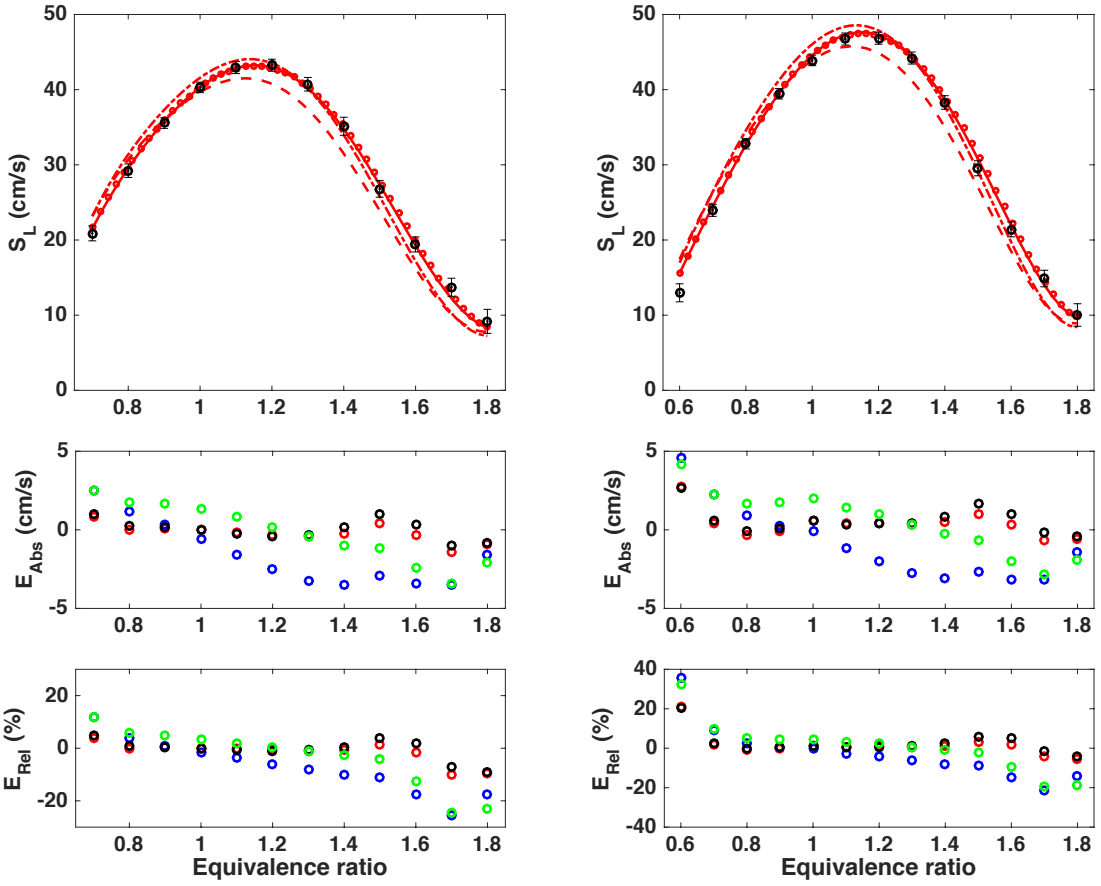
a) Major species b) Minor species

c) Major species d) Minor species

Figure 3: Comparison between the experimental [1] and the predicted species profiles for acetaldehyde-oxygen-nitrogen mixtures in a jet stirred reactor. Conditions in a) and b): Φ=0.09; X_{N2}=0.96117; P=101 kPa; residence time=0.08 s. Conditions in c) and d): Φ=1.61; X_{N2}=0.996925; P=101 kPa; residence time=0.08 s.

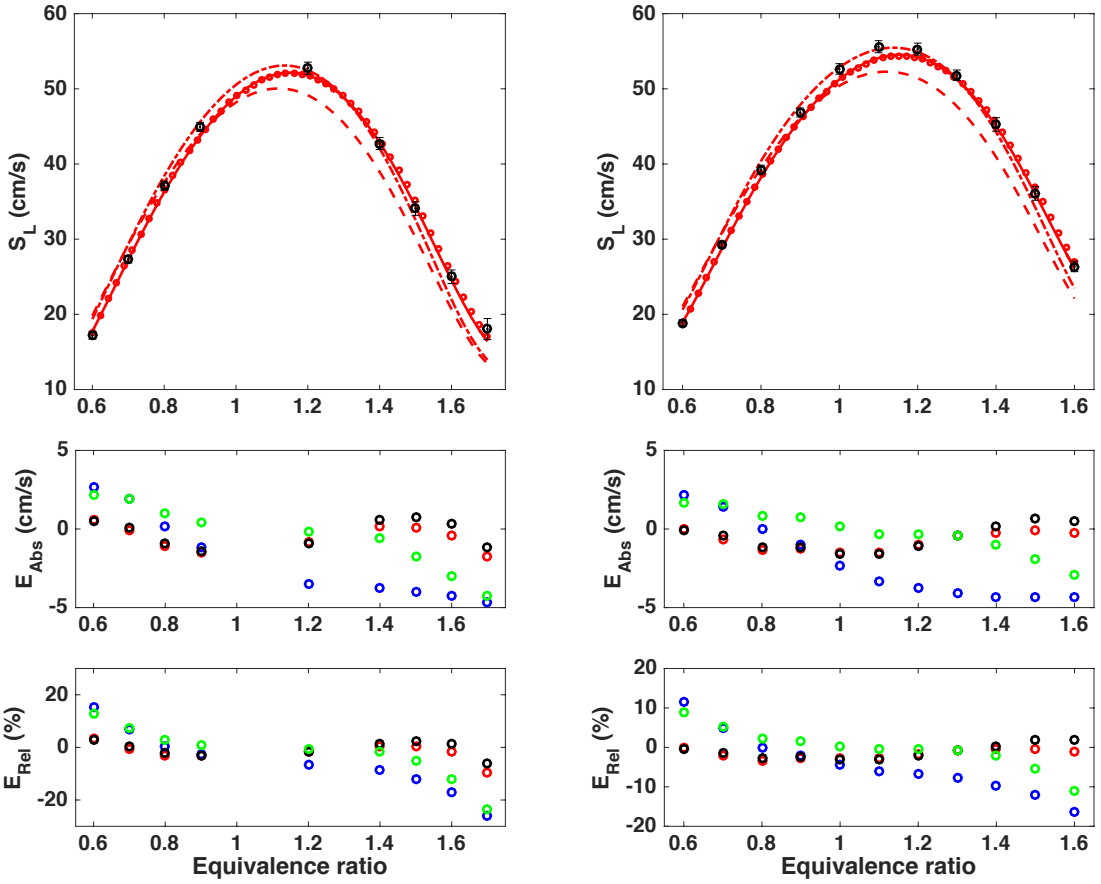
Laminar flame speed

Laminar flame speed data from Christensen et al. study [2] have been modeled using the freely-propagating flame code from Cantera. Note that the experimental values from [2] have been multiplied by 1.055 as recommended in Alekseev et al. [3]. Figure 4 shows a comparison between the experimental flame speed and the predictions of the four models previously used. The absolute and relative errors are also indicated.



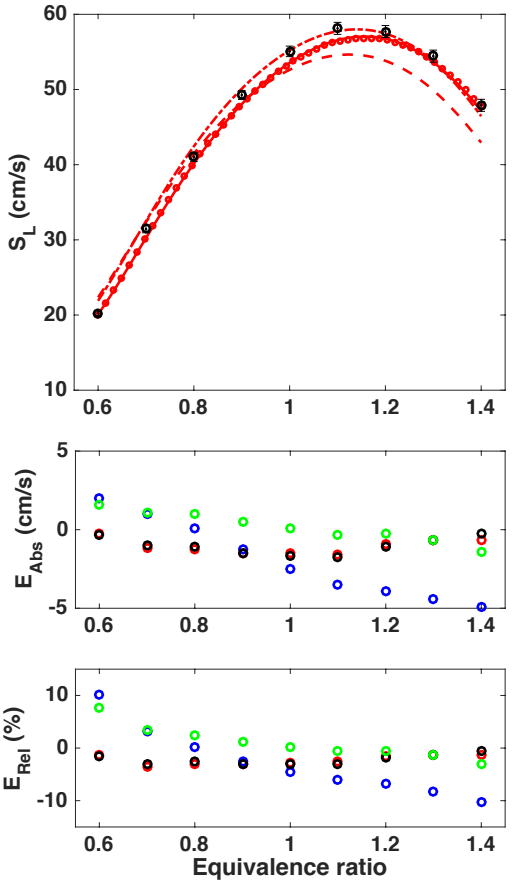
a) P=101 kPa and T=298 K b) P=101 kPa and T=318 K

Figure 4: Comparison between the experimental [2, 3] and the predicted laminar flame speed for acetaldehyde-air mixtures. For absolute and relative errors: red circles: present model; green circles: Aramco 2.0; black circles: CaltechMech; blue circles: JetSurf.



a) P=101 kPa and T=338 K b) P=101 kPa and T=348 K

Figure 5: Comparison between the experimental [2, 3] and the predicted laminar flame speed for acetaldehyde-air mixtures. For absolute and relative errors: red circles: present model; green circles: Aramco 2.0; black circles: CaltechMech; blue circles: JetSurf.

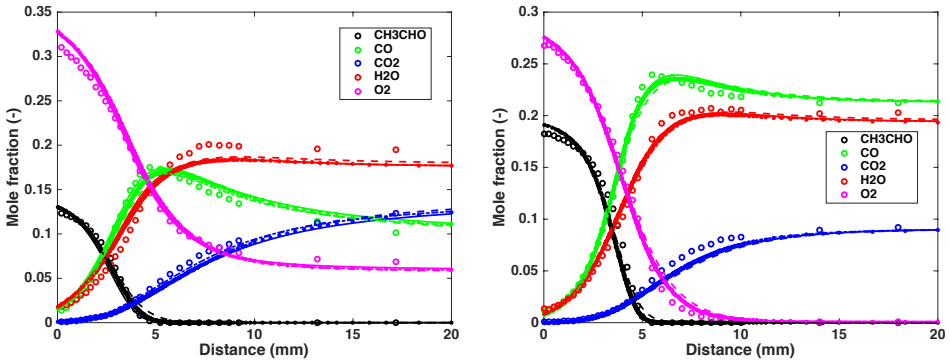


P=101 kPa and T=358 K

Figure 6: Comparison between the experimental [2, 3] and the predicted laminar flame speed for acetaldehyde-air mixtures. For absolute and relative errors: red circles: present model; green circles: Aramco 2.0; black circles: CaltechMech; blue circles: JetSurf.

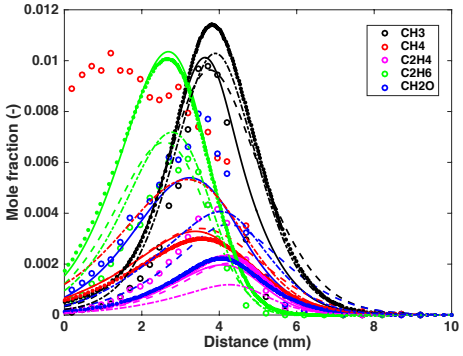
Flame structure

Flame structure data from Tao et al. study [4] have been modeled using the flat flame code from Cantera. Figure 7 shows a comparison between the experimental profiles for the major species and the predictions of the four models previously used.

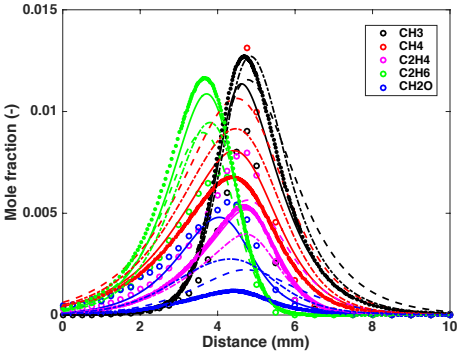


a) Major species for Φ=1

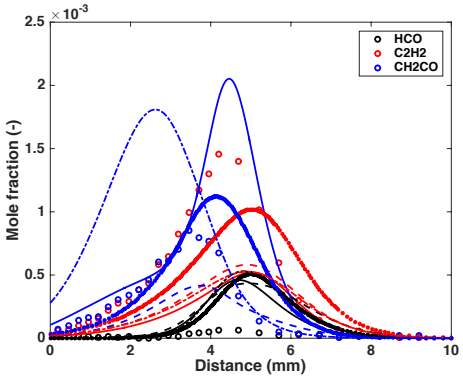
b) Major species for Φ=1.7



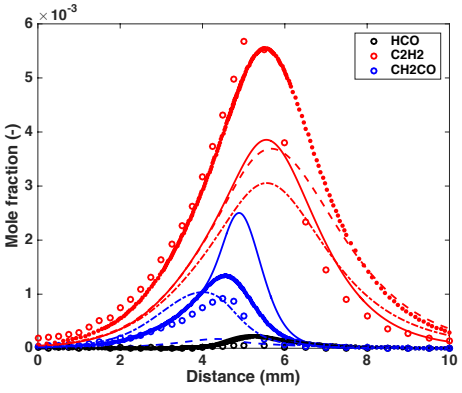
c) Minor species for Φ=1



d) Minor species for Φ=1.7



e) Minor species for Φ=1



f) Minor species for Φ=1.7

Figure 7: Comparison between the experimental [4] and the predicted species profiles in low-pressure acetaldehyde-oxygen-argon flat flames. Conditions in a), c), e): Φ=1; P=2 kPa; X_{Ar}=0.5. Conditions in b), d) and f): Φ=1.7; P=4 kPa; X_{Ar}=0.5.

References

[1] P. Dagaut, M. Reuillon, D. Voisin, M. Cathonnet, M. M. Guinness, J. Simmie, Combustion Science and Technology 107 (1995) 301–316.

[2] M. Christensen, M. Abebe, E. Nilsson, A. Konnov, Proceedings of the Combustion Institute 35 (2015) 499 – 506.

[3] V. Alekseev, J. Naucler, M. Christensen, E. Nilsson, E. Volkov, L. de Goey, A. Konnov, Combustion Science and Technology 188 (2016) 853–894.

[4] T. Tao, W. Sun, B. Yang, N. Hansen, K. Moshammer, C. Law, Proceedings of the Combustion Institute In press (2016).