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What should be the target theme of ISF5?

Inception, surface growth, oxidation, particle morphology and coagulation, soot yield or soot optical properties?

We could focus on soot yield and morphology because by accurately simulating these two, models need to accurately account for the balance between inception, surface growth, oxidation and coagulation. Thus, we can set flames/reactors that provide such information as targets.

Potential Target Flames for ISF 5
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Premixed Flames

1. ISF4-premixed 1a (Ethylene/Air flame)- has the most comprehensive dataset, *"ISF-5 main"*

1.1. Reason for choosing:

a. Multiple consistent experiments (with different methods) [1, 2, ISF website] and simulations (1D and 2D [3]) from different groups are available.
b. In addition to 1a, there is data available for a series of flames at different equivalence rations and cold gas velocities, $\varphi = 2.07, 3.21 \leq v_0 \leq 5.88\ {}^{cm}/_{s}$ and $\varphi = 2.16, 2.94 \leq v_0 \leq 6.15\ {}^{cm}/_{s}$ [ISF website].

1.2. Flame conditions:

a. Ethylene/Air flame, $\varphi = 2.07, C/O = 0.69, v_0 = 5.87\ {}^{cm}/_{s}$

1.3. Available data:

a. Soot volume fraction, f_v, measured optically by Laser extinction (632 nm) [1, ISF website from 4 and 5], two color pyrometry [1], and intrusively by SMPS [1, 2].
b. Soot agglomerate number density [1,2, ISF website from 4 and 5].
c. Particle size distributions measured by SMPS [1]
d. Species concentrations up to 3-ring aromatics [1] as well as 6 ring aromatics [upcoming from Sandro Gomez group from Yale].
e. Soot size data from light scattering [upcoming from Sandro Gomez group from Yale].
f. no morphology data is available from TEM images.
g. no particle mass data is available from CPMA or APM.

1.4. References:

1. Carbone, F et al, 2017. *Combust Flame*, *181*, 315-328
2. Maricq, M.M., 2004. *Combust Flame*, *137*, 340-350.
3. Xuan, Y. and Blanquart, G., 2016. *Combust Flame*, *166*, 113-124.
4. H. Bohm, D. Hesse, H. Jander, B. Luers, J. Pietscher, H. GG. Wganer, M. Weiss, Proc. Comb. Inst. 22 (1988) 403-411
5. H. Matzing, H. Gg. Wagner, Proc. Comb. Inst. 21 (1986) 1047-1055.
6. F. Carbone, et al., Proc. Combust. Inst. 37 (2019) 919–926.
7. F. Carbone, S. Moslih, A. Gomez, Combust. Flame 181 (2017) 329–341.
8. F. Carbone, M. Attoui, A. Gomez, Aerosol Sci. Technol. 50 (2016) 740–757.

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2. ISF4-premixed 3 (Ethylene/Air flame) (LII target flames):
"ISF-5 main"

2.1. Reason for choosing:

a. Optical data available from multiple groups for soot volume fraction with LII [1, 3, 4, 5] and LE using different wavelengths [3, 4, 7, 8, 9]
b. Soot morphology (primary particle diameter) is available from TEM images [7, 8] as well as light scattering [7, 8] and LII [1]
c. In addition to 3a, there is data available for a series of flames at different equivalence rations, $\varphi = 2.1, 2.31, 2.5$.

2.2. Flame conditions:

a. Ethylene/Air flame, $\varphi = 2.1, C/O = 0.7, v_0 = 6.37\ {}^{cm}/_{s}$
   And $\varphi = 2.31, C/O = 0.77, v_0 = 6.37\ {}^{cm}/_{s}$

2.3. Available data:

a. Soot volume fraction, f_v, measured optically by Laser extinction 405 to 1064 nm and LII.
b. Soot primary particle [7, 8], d63, d30 (volume equivalent diameter) and gyration diameters are available.
c. Flame temperature with CARS [2]
d. No species concentrations are available.
e. No particle size distributions are available.
f. no particle mass data is available from CPMA or APM.

2.4. References

1. B. Axelsson, R. Collin, P.-E. Bengtsson, Appl. Opt. 39 (2000) 3683-3690.
2. C. Brackmann, J. Bood, P.-E. Bengtsson, T. Seeger, M. Schenk, A. Leipertz, Appl. Opt. 41 (2002), 564-572.
3. F. Migliorini, S. De Iuliis, F. Cignoli, G. Zizak, Comb. Flame 153 (2008) 384-393
4. J. Zerbs, K.P. Geigle, O. Lammel, J. Hader, R. Stirn, R. Hadef, W. Meier, Appl. Phys. B 96 (2009), 683-694.
5. R. Hadef, K.P. Geigle, W. Meier, M. Aigner, Int. J. Thermal Sci. 49 (2010) 1457-1467.
6. H. Bladh, J. Johnsson, N.-E. Olofsson, A. Bohlin, P.-E. Bengtsson, Proc. Comb. Inst. 33 (2011) 641-648.
7. S. De Iuliis, S. Maffi, F. Cignoli, G. Zizak, Appl. Phys. B 102 (2011) 891-903.
8. S. De Iuliis, S. Maffi, F. Migliorini, F. Cignoli, G. Zizak, Appl. Phys. B 106 (2012) 707-715.
9. Simonsson, J., Olofsson, N.E., Török, S., Bengtsson, P.E. and Bladh, H., 2015. *Applied Physics B*, *119*(4), pp.657-667.

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3. (NEW) ISF5-premixed (Jet A doped into an Ethylene/Oxygen/Nitrogen host flame)

3.1. Reason for Choosing:

a. Sooting flame data for real jet fuel (POSF-10325) and the 2nd generation MURI surrogate [1].
b. Detailed particle size distributions are available for a series of flames with different cold gas velocities [1].
c. Data is also available for counterflow and coflow diffusion flames [1].

3.2. Flame Conditions:

a. **Stretch-stabilized stagnation** ethylene-oxygen-nitrogen host flame (12.2% C_2H_4 - 17.8% O_2 - 70.0% N_2, Φ=2.06) doped with 7300 ppm by mass (Φ=2.18) and 11500 ppm by mass (Φ=2.24) of jet fuel, or the 2nd generation MURI surrogate.
b. Three different cold gas velocities to probe different particle residence times in the flames.

3.3. Data Available:

a. Soot volume fraction (SMPS).
b. Particle size distributions (SMPS).
c. No species concentrations are available.
d. No soot concentration from optical diagnostics is available.
e. No particle morphology data from TEM analysis is available.
f. no particle mass data is available from CPMA or APM.

3.4. References:

1. Saggese, C., Singh, A.V., Xue, X., Chu, C., Kholghy, M.R., Zhang, T., Camacho, J., Giaccai, J., Miller, J.H., Thomson, M.J. and Sung, C.J., 2019. The distillation curve and sooting propensity of a typical jet fuel. *Fuel*, *235*, pp.350-362.

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4. *ISF4-premixed 6* (Ethylene/Argon/Oxygen flame) *(benchmarked premixed flame)*

4.1. Reason for choosing:

a. Detailed particle size distributions are available for a series of flames from multiple groups [1]
b. Soot mass mobility measurements from CPMA are available [1]
c. Soot primary particle data is available from HIM [1,2]
d. Simulated by multiple groups using 1D and 2D approaches [3,4]

4.2. Flame Conditions:

a. Ethylene, Argon, oxygen flame, $\varphi = 2.07, C/O = 0.69, v_0 = 8\ {}^{cm}/_{s}$

4.3. Available data:

a. Particle size distributions with SMPS [1].
b. Particle mass with CPMA [1].
c. SMPS agglomerate number density and volume fraction [1].
d. Some particle morphology data is available from TEM analysis [5].
e. No species concentrations are available.
f. No soot concentration measured by optical diagnostics is available.

4.4. References:

1. Camacho, J., Liu, C., Gu, C., Lin, H., Huang, Z., Tang, Q., You, X., Saggese, C., Li, Y., Jung, H. and Deng, L., 2015. Mobility size and mass of nascent soot particles in a benchmark premixed ethylene flame. *Combustion and Flame*, *162*, 3810-3822.

2. Saggese, C., Ferrario, S., Camacho, J., Cuoci, A., Frassoldati, A., Ranzi, E., Wang, H. and Faravelli, T., 2015. Kinetic modeling of particle size distribution of soot in a premixed burner-stabilized stagnation ethylene flame. *Combustion and Flame*, *162*(9), pp.3356-3369.

3. Saggese, C., Cuoci, A., Frassoldati, A., Ferrario, S., Camacho, J., Wang, H. and Faravelli, T., 2016. Probe effects in soot sampling from a burner-stabilized stagnation flame. *Combustion and Flame*, *167*, pp.184-197.

4. Kelesidis, G.A., Kholghy, M.R., Zuercher, J., Robertz, J., Allemann, M., Duric, A. and Pratsinis, S.E., 2019. Light scattering from nanoparticle agglomerates. *Powder Technology*.

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5. ***(NEW) ISF5-premixed 1*** (Methane/Oxygen/Nitrogen) ("nucleation" and "growth" low pressure methane flames)

5.1. Reason for choosing:

a. These flames could be used for calibrating nucleation models [4]
b. Detailed species data and LII Fv and dp data are available [2].
c. Modeling both flames with identical parameters is challenging [1,4]

5.2. Flame Conditions:

a. Methane, Oxygen, Nitrogen flames:

"nucleation", $\varphi = 1.95, C/O = 0.49,\ \dot{m} = 25.681\ \frac{g}{m^2 \cdot s}$

"growth" , $\varphi = 2.32, C/O = 0.58,\ \dot{m} = 25.698\ \frac{g}{m^2 \cdot s}$

5.3. Available data:

a. Temperature measurements with different methods [3].
b. Species concentrations on Naphtalene (upcoming data from Lille) Pyrene and fluoranthene [1].
c. Soot volume fraction and primary particles with LII [1].
d. Soot bulk and surface H/C data for the growth flame [upcoming from Lille].
e. No particle size distributions are available.
f. No soot size data from intrusive methods (TEM) are available.
g. no particle mass data is available from CPMA or APM.

5.4. References:

1. Desgroux, P., Faccinetto, A., Mercier, X., Mouton, T., Karkar, D.A. and El Bakali, A., 2017. *Combustion and Flame*, *184*, 153-166.
2. Mouton, T., Mercier, X. and Desgroux, P., 2016. Isomer discrimination of PAHs formed in sooting flames by jet-cooled laser-induced fluorescence: application to the measurement of pyrene and fluoranthene. *Applied Physics B*, *122*(5), p.123.
3. Burns, I.S., Mercier, X., Wartel, M., Chrystie, R.S., Hult, J. and Kaminski, C.F., 2011. A method for performing high accuracy temperature measurements in low-pressure sooting flames using two-line atomic fluorescence. *Proceedings of the Combustion Institute*, *33*(1), pp.799-806.
4. Aubagnac-Karkar, D., El Bakali, A. and Desgroux, P., 2018. Soot particles inception and PAH condensation modelling applied in a soot model utilizing a sectional method. *Combustion and Flame*, *189*, pp.190-206.

6. ***(NEW) ISF5-premixed 2*** (n-butane, Oxygen, Nitrogen flames)-has a complete dataset. ("nucleation" and "growth" n-butane 1 atm flames):

6.1. Reason for choosing:

a. Soot volume fraction and size data with multiple techniques are available [1,2].
b. Particle size distribution with SMPS as well as HIM [1].
c. Detailed species measurements [upcoming from Lille].

6.2. Flame conditions:

a. n-butane, Oxygen, Nitrogen flames, nucleation (φ =1.75), growth flame (φ =1.95), and a non-sooting flame (φ =1.6)

6.3. Data available:

a. Particle morphology and primary particle diameter (HIM) [1]
b. Particle mobility size distribution (1-nm SMPS) [1, upcoming from Lille]
c. Soot volume fraction (LII calibrated by cavity ring down extinction) [1,2]
d. Primary particle diameter estimated by LII
e. Species concentrations, C_2H_2, C_6H_6, $C_{10}H_8$ and $C_{16}H_{10}$ [upcoming from Lille]
f. Measured temperature profiles [1]
g. no particle mass data is available from CPMA or APM.

6.4. References:

1. Betrancourt, C., Liu, F., Desgroux, P., Mercier, X., Faccinetto, A., Salamanca, M., Ruwe, L., Kohse-Höinghaus, K., Emmrich, D., Beyer, A. and Gölzhäuser, A., 2017. Investigation of the size of the incandescent incipient soot particles in premixed sooting and nucleation flames of n-butane using LII, HIM, and 1 nm-SMPS. *Aerosol Science and Technology*, *51*(8), pp.916-935.
2. Betrancourt, C., Mercier, X., Liu, F. and Desgroux, P., 2019. Quantitative measurement of volume fraction profiles of soot of different maturities in premixed flames by extinction-calibrated laser-induced incandescence. *Applied Physics B*, *125*(1), p.16.

Counterflow Diffuion Flames

1. (new) ISF 5 Counterflow 1, *"ISF-5 main"-only the green ones*

1.1. Reason for Choosing:

a. Has species concentrations up to 6-ring aromatics as well as soot concentration and size.
b. A series of flames with different pressures and strain rates are available.

1.2. Flame Conditions:

P (atm)	C_2H_4 mol frac.	Zst	Global strain rate (s^{-1})	Published Data	Ref.	Unpublished Data
1	0.122	0.408	57	GC (up to 2-rings)	[1]	
2	0.122	0.408	57	GC (up to 2-rings)	[1]	
4	0.122	0.408	57	GC (up to 2-rings)	[1]	
8	0.122	0.408	57	GC (up to 2-rings)	[1]	
2.9	0.0975	0.408	18	GC (up to 2-rings)	[2]	
8.5	0.0975	0.408	18	GC (up to 2-rings)	[1]	
25	0.0975	0.408	18	GC (up to 2-rings)	[1,2]	
1	0.330	0.183	50	GC (up to 3-rings), soot vol. frac.	[3,5]	GC (up to 6-rings), Soot particle size
4	0.255	0.183	50	GC (up to 3-rings), soot vol. frac.	[4,6]	GC (up to 6-rings), Soot particle size
8	0.225	0.183	50	GC (up to 3-rings)	[4,6]	GC (up to 6-rings)

P (atm)	C_2H_4 mol frac.	Zst	Global strain rate (s^{-1})	Published Data	Current Work
16	0.225	0.183	50	N/A	GC, Soot vol frac. & size
8	0.114	0.408	18	N/A	GC, Soot vol frac. & size
16	0.110	0.408	18	N/A	GC, Soot vol frac. & size
32	0.102	0.408	18	N/A	GC, Soot vol frac. & size

1.3. Data Available

As listed above.

1.4. References:

1. L. Figura, A. Gomez, Combust. Flame 161 (2014) 1587–1603.
2. L. Figura, F. Carbone, A. Gomez, Proc. Combust. Inst. 35 (2015) 1871–1878.
3. F. Carbone, F. Cattaneo, A. Gomez, Combust. Flame 162 (2015) 4138–4148.
4. F. Carbone, K. Gleason, A. Gomez, Proc. Combust. Inst. 36 (2017) 1395–1402.
5. K. Gleason, F. Carbone, A. Gomez, Combust. Flame 192 (2018) 283–294.
6. K. Gleason, F. Carbone, A. Gomez, Proc. Combust. Inst. 37 (2019) 2057–2064.

2. (New) ISF 5 Counterflow 2: (Fuel: C2H2, CH4, C3H6O, CO2)

2.1. Reason for choosing the flame:

a. Detailed species measurements are available for very low sooting conditions.

2.2. Flame conditions:

a. Series of atmospheric counterflow flames with a strain rate of 70 1/s and comparable stoichiometric mixture fractions and equilibrium temperature. Following a progressive approach, the first flame is an argon-diluted counterflow flame (ACAir), the second (AcOxyFlame) includes also carbon dioxide on both sides to simulate oxy-fuel conditions, additionally methane (AcMeOxy) is added to reproduce a typical light-volatiles mixtures of coal and biomass.

2.3. Data Available:

a. Species profiles by Time-of-Flight (ToF) for fuel, oxidizer and C_3H_5, CH_3, C_2H_3, C_4H_8, C_5H_6, C_5H_8, C_3H_3, C_6H_6 as well as PAH concentration such as (C_7H_8, C_8H_6, C_8H_8, C_9H_8, $C_{10}H_8$)
b. No soot measurements are available as flames produce low amounts of soot.

2.4. References:

1. Baroncelli, M., Felsmann, D., Hansen, N. and Pitsch, H., 2019. Investigating the effect of oxy-fuel combustion and light coal volatiles interaction: A mass spectrometric study. *Combustion and Flame*, *204*, pp.320-330.

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3. (New) ISF 5 Counterflow 2: (Fuel: C_2H_4, iso-octane, n-heptane, toluene)

3.1. Reason for choosing the flame:

a. soot measurements in iso-octane, n-heptane, toluene, and ethylene counterflow flames over a range of mass fractions and strain rates for each fuel

3.2. Flame conditions:

a. Series of atmospheric counterflow flames with a strain rate of 70 1/s and comparable stoichiometric mixture fractions and equilibrium temperature. Following a progressive approach, the first flame is an argon-diluted counterflow flame (ACAir), the second (AcOxyFlame) includes also carbon dioxide on both sides to simulate oxy-fuel conditions, additionally methane (AcMeOxy) is added to reproduce a typical light-volatiles mixtures of coal and biomass.

3.3. Data Available:

a. Only soot volume fraction measurements with LII calibrated by LE.
b. Species measurements are planned. The flames might be too sooty for sampling techniques. Therefore, boundary conditions might slightly be varied.
c. No size distribution data is available
d. No morphology data from TEM analysis is available

3.4. References:

1. Upcoming from Aachen

4. (new) ISF 5 Counterflow 3: (Jet A doped into an Ethylene/Oxygen/Nitrogen host flame) from Stanford/UCONN

4.1. Reason for choosing:

a. Sooting flame data for real jet fuel and its light and heavy distillate fractions
b. Data is also available for premixed and coflow flames.

4.2. Flame conditions:

a. The host counterflow diffusion flames were established with a fuel stream of C_2H_4/N_2 flowing against an oxidizer stream of O_2/N_2.
b. The nozzle to nozzle separation distance is 1.1 cm
c. The global strain rate was maintained at K=200 s^{-1}.
d. The mole fraction of C_2H_4 in the fuel stream, X_F, and the mole fraction of O_2 in the oxidizer stream, XO_2, were kept equal. There are three series of flames: two sooting conditions, $X_F= X_{O2}=0.40$ and $X_F= X_{O2}=0.35$, and one near-sooting condition of $X_F= X_{O2}=0.30$, which were selected for the host flames.
e. Jet A or a certain distillate fraction was doped into the fuel stream at the concentration of 2000 ppm by mole. In the doped flames, the ethylene mole fraction was slightly reduced and accordingly to keep the total fuel mole fraction and thus the total fuel jet velocity the same between the doped and host flames.
f. Fuel and oxidizer streams were maintained at 400 K.
g. Both fuel and oxidizer cold gas velocities are 56 cm/s.

4.3. Available data:

a. Soot volume fraction (LII) [1]
b. No species data is available
c. No size distribution data is available
d. No morphology data from TEM analysis is available

4.4. References:

1. Saggese, C., Singh, A.V., Xue, X., Chu, C., Kholghy, M.R., Zhang, T., Camacho, J., Giaccai, J., Miller, J.H., Thomson, M.J. and Sung, C.J., 2019. The distillation curve and sooting propensity of a typical jet fuel. *Fuel*, *235*, pp.350-362.

5. (new) ISF 5 Counterflow 4, KAUST1

5.1. Reason for choosing

a. Investigated the impact of strain rate on soot concentration
b. Has soot volume fraction, number density and d63

5.2. Flame conditions

a. The nozzle exit velocities (*V_0*) tested were 10, 15, 20, 25 and 30 cm/s,

5.3. Available data

a. Soot volume fraction, particle size (D63) and number density
b. No species data is available
c. No size distribution data is available
d. No morphology data from TEM is available

5.4. References

1. Wang, Y., & Chung, S. H. (2016). Strain rate effect on sooting characteristics in laminar counterflow diffusion flames. *Combustion and Flame*, *165*, 433-444.
2. Joo, P.H., Wang, Y., Raj, A. and Chung, S.H., 2013. Sooting limit in counterflow diffusion flames of ethylene/propane fuels and implication to threshold soot index. *Proceedings of the Combustion Institute*, *34*(1), pp.1803-1809.

6. (NEW) ISF 5 Counterflow 5, KAUST2

6.1. Reason for choosing

a. Data available for flames at different pressures
b. Optical and TEM data are also available

6.2. Flame conditions

a. high pressures up to 10 atm
b. air, ethylene and nitrogen with mixture fractions of Z_{st} = 0.253 and 0.184 [2]
c. constant global strain rate of 30 1/s [2]

6.3. Available data

a. Soot volume fraction, primary particle number density, agglomerate number density,
b. primary particle diameter (TEM) and distribution (TEM) and agglomerate radius of gyration.

6.4. References

1. Amin, H.M. and Roberts, W.L., 2017. Soot measurements by two angle scattering and extinction in an N2-diluted ethylene/air counterflow diffusion flame from 2 to 5 atm. *Proceedings of the Combustion Institute*, *36*(1), pp.861-869.
2. Amin, H.M., Bennett, A. and Roberts, W.L., 2019. Determining fractal properties of soot aggregates and primary particle size distribution in counterflow flames up to 10 atm. *Proceedings of the Combustion Institute*, *37*(1), pp.1161-1168.

7. (NEW) ISF 5 Counterflow 6, Virginia (ethylene/oxygen/inert)

7.1. Reason for choosing

a. Has data for a series of flames with different strain rates and pressures.
b. Measured soot volume fraction, primary particle diameter (LII), and number density (I guess it is primary particle number density calculated based on volume fraction and LII dp)

7.2. Flame conditions

7.3. Available data

a. Soot volume fraction, primary particle size and number density from LII
b. No species data
c. No morphology data from TEM is available

7.4. References

1. Sarnacki, B.G. and Chelliah, H.K., (2018). Sooting limits of non-premixed counterflow ethylene/oxygen/inert flames using LII: Effects of flow strain rate and pressure (up to 30 atm). *Combustion and Flame*, *195*, 267-281.

Coflow Diffuion Flames

<u>1. ISF4-Coflow 1a (Ethylene/Air non-smoking flame)</u>

1.1. Reason for choosing:

a. Has the most comprehensive dataset

1.2. Flame conditions:

a. Ethylene Sooting Flame Nonsmoking
b. Fuel: Ethylene, Oxidizer: Air
c. Fuel flow rate: 3.85 cm3/s, Fuel velocity: 3.98 cm/s
d. Oxidizer flow rate: 713.3 cm3/s, Oxidizer velocity: 8.90 cm/s

1.3. Available data:

a. Integrated soot volume fraction as a function of height.
b. Soot volume fraction along the centreline, wings, and selected radial cuts
c. Primary particle number density, particle number density, and primary particle diameter along the max soot line
d. T, C2H2, OH at select radial cuts
e. T along the flame centerline
f. Max T at each height
g. Soot particle TEM images
h. No size distributions is available

1.4. References:

1. R.J. Santoro, H.G. Semerjian, R.A. Dobbins, Combust. Flame, 51, (1983) 203-218.
2. R.J. Santoro, T.T. Yeh, J.J. Horvath, H.G. Semerjian, Combust. Sci. Technol. 53 (1987) 89-115.
3. C.M. Megaridis, R.A. Dobbins, Proc. Combust. Inst. 22 (1988) 353-362.
4. C.M. Megaridis, R.A. Dobbins, Combust. Sci. Technol. 66 (1989) 1-16.
5. R. Puri, T.F. Richardson, R.J. Santoro, R.A. Dobbins, Combust. Flame 92 (1993) 320-333.
6. I.M. Kennedy, C. Yam, D.C. Rapp, R.J. Santoro, Combust. Flame, 107 (1996) 368-382.
7. C.S. McEnally, U.O. Köylü, L.D. Pfefferle, D.E. Rosner, Combust. Flame, 109 (1997) 701-720.
8. U.O. Köylü, C.S. McEnally, D.E. Rosner, L.D. Pfefferle, Combust. Flame, 110 (1997) 494-507.
9. A.G. Yazicioglu, C.M. Megaridis, A. Campbell, K.O. Lee, M.Y. Choi, Combust. Sci. Technol. 171 (2001) 71-87.
10. S.S. Iyer, T.A. Litzinger, S.Y. Lee, R.J. Santoro, Combust. Flame 149 (2007) 206-216.
11. C.P. Arana, M. Pontoni, S. Sen, I.K. Puri, Combust. Flame 138 (2004) 362–372.
12. Kholghy, M.R., Veshkini, A. and Thomson, M.J., 2016. The core–shell internal nanostructure of soot–a criterion to model soot maturity. *Carbon*, *100*, pp.508-536.

2. **ISF4-Coflow 3 (Ethylene/Air** non-smoking, diluted with varying levels of nitrogen**)** ***"ISF-5 main"***

2.1. Reason for choosing:

a. Flames have well documented boundary conditions

2.2. Flame conditions:

b. non-smoking Ethylene Sooting flame, fuel diluted with different amounts of nitrogen,
c. Fuel: Ethylene/N_2. Fuel velocity: 35 cm/s (cold-flow velocity), Fuel flow rate: 4.4 cm3/s (STP)
d. Oxidizer: Air, Oxidizer velocity: 35 cm/s (cold-flow velocity), Oxidizer flow rate: 687.16 cm3/s (STP)

2.3. Available data:

a. Temperature isotherms
b. Benzene concentration isopleths
c. Soot volume fraction isopleths
d. Soot volume fraction at selected radial cuts
e. T at selected radial cuts
f. T, C2H2 and benzene along the flame centerline
g. Soot temperature contour
h. Some diameter measurements from TEM

2.4. References:

1. Smooke MD, Long MB, Connelly BC, Colket MB, Hall RJ. Combustion and Flame 2005;143(4):613–28
2. M.D. Smooke, R.J. Hall, M.B. Colket, et al, J. Fielding, M.B. Long, C.S. McEnally, and L.D. Pfefferle, Combust. Theory Model. 8 (2004) 593–606.
3. Kuhn, P.B., Ma, B., Connelly, B.C., Smooke, M.D., Long, M.B., (2011) Proceedings of the Combustion Institute, 33 (1), pp. 743-750.
4. Herdman, J.D., Connelly, B.C., Smooke, M.D., Long, M.B., Miller, J.H., (2011) Carbon, 49 (15), pp. 5298- 5311.
5. Kempema, N.J. and Long, M.B., 2018. Effect of soot self-absorption on color-ratio pyrometry in laminar coflow diffusion flames. *Optics letters*, *43*(5), pp.1103-1106.
6. Botero, M.L., Eaves, N., Dreyer, J.A., Sheng, Y., Akroyd, J., Yang, W. and Kraft, M., 2019. Experimental and numerical study of the evolution of soot primary particles in a diffusion flame. *Proceedings of the Combustion Institute*, *37*(2), pp.2047-2055.
7. Kholghy, M.R., Eaves, N.A., Veshkini, A. and Thomson, M.J., 2019. The role of reactive PAH dimerization in reducing soot nucleation reversibility. *Proceedings of the Combustion Institute*, *37*(1), pp.1003-1011.

3. ISF4- linked co-flow flames 2: Santoro-Adelaide burner data

3.1. Reason for choosing:

3.2. Flame conditions:

Non-smoking, co-flowing ethylene/hydrogen/nitrogen flames. Linked to turbulent flames: ISF-3 target flame 1 (Adelaide Jet Flames 1-6). There are two series of flames:

a. Flame set-I: the flow rate of ethylene is held constant as 0.207 Liters/minute, corresponding to an exit velocity of 0.040 m/s, while hydrogen or nitrogen is added to the fuel at a volumetric fraction of 20% or 40%, also including a pure ethylene flame (ethylene: 0.207 L/min).
b. Flame set-II: the total flow rate of ethylene/hydrogen/nitrogen mixture is held constant as 0.259 Liters/minute, corresponding to an exit velocity of 0.050 m/s, while the volumetric fractions of ethylene, hydrogen and nitrogen are varied (from 0 to 40%), also including a pure ethylene flame (ethylene: 0.259 L/min)

3.3. Available data:

a. Soot volume fraction (LII), primary particle diameter (LII), flames temperature were measured with planar optical methods. Flame temperature was also measured with a thermocouple in the upstream of the flames.
b. No soot morphology from TEM analysis is available

3.4. References:

1. Sun, Z., Dally, B., Nathan, G. and Alwahabi, Z., 2017. Effects of hydrogen and nitrogen on soot volume fraction, primary particle diameter and temperature in laminar ethylene/air diffusion flames. *Combustion and Flame*, *175*, pp.270-282.

Laminar Flow Reactors

1. ISF5-Laminar Flow Reactor (Methane/Oxygen diluted with nitrogen)

1.1. Reason for choosing:

a. Rich collection of gas-phase species measurements, particle volume fraction, particle density, and mean particle diameter for wide temperature range.
b. This data is suitable for testing oxidation models and effect of temperature.

1.2. Flame conditions:

a. Fuel: Methane/Oxygen/N2. Inlet flow rates: 5 Nl/min
b. Reactor temperatures: 1073 – 1823 K

1.3. Available data:

c. Axial Temperature Profiles
d. Gas-phase species measurements: O_2, CO, CO_2, CH_4, C_2H_6, C_2H_2, and C_6H_6
e. PAH measurements: styrene, biphenyl, naphthalene, indene, acenaphthalene, phenanthrene, pyrene
f. Particle volume fraction and density measurements using filters
g. Particle mean mobility diameter measurements using SMPS
h. no morphology data is available from TEM images.
i. no particle mass data is available from CPMA or APM.

1.4. References:

1. M.S Skjøth-Rasmussen, P Glarborg, M Østberg, J.T Johannessen, H Livbjerg, A.D Jensen, T.S Christensen, Combustion and Flame, 2004; 136 (1–2), 91-128
2. Ali Naseri, Murray J. Thomson, Combustion and Flame, 2019; 207, 314-326

2. ISF5-Laminar Flow Reactor (Ethylene diluted with nitrogen)

2.1. Reason for choosing:

a. Inclusion of both PSD profiles and SEM images of the particles provide a unique opportunity to assess the aggregate structure prediction of the models.

2.2. Flame conditions:

a. Fuel: Ethylene/N2. Inlet flow rates: 2 – 7 Nl/min
b. Reactor temperatures: 1600 – 1800 K

2.3. Available data:

a. Axial Temperature Profiles
b. Particle Size distribution (PSD) measurements
c. Some SEM images of the particles
d. no morphology data is available from TEM images.
e. no particle mass data is available from CPMA or APM.

2.4. References:

1. Kazuki Dewa, Kiminori Ono, Aki Watanabe, Kaname Takahashi, Yoshiya Matsukawa, Yasuhiro Saito, Yohsuke Matsushita, Hideyuki Aoki, Koki Era, Takayuki Aoki, Togo Yamaguchi, Combustion and Flame, 2016; 163, 115-121
2. Ali Naseri, Murray J. Thomson, Combustion and Flame, 2019; 207, 314-326

3. ISF5-Laminar Flow Reactor (Ethylene, Ethane, Ethanol diluted with nitrogen)

3.1. Reason for choosing:

a. The particle mass provided in this data set is ideal to test the mass closure of the particle formation models.

3.2. Flame conditions:

a. Fuel: Ethylene, Ethane, Ethanol/N2. Inlet flow rates: 20 l/min
b. Reactor temperatures: 1000 – 1400 °C

3.3. Available data:

a. Particle size distribution measurements with SMPS
b. Total particle mass measurements using filter

3.4. References:

1. A. Eveleigh, N. Ladommatos, R. Balachandran, Energy Procedia, 2015; 66, 41-44

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4. ISF5-Laminar Flow Reactor (Ethylene, diluted with nitrogen)

4.1. Reason for choosing:

a. A comprehensive data set to study the effect of the inlet fuel mole fractions, flow rate, and the reactor temperature on the shape of the PSD profiles.

4.2. Flame conditions:

a. Fuel: Ethylene/N2: X_{C2H2}=0.4, 0.6, 0.8; Inlet flow rates: 7 to 15.5 l/min
b. Reactor temperatures: 1573, 1673, 1773 K

4.3. Available data:

a. Axial temperature profiles
b. Particle size distribution (PSD) measurements using SMPS
c. Total count of particle using SMPS
d. no morphology data is available from TEM images.
e. No yield data
f. no particle mass data is available from CPMA or APM.

4.4. References:

1. Junyu Mei, Mengda Wang, Xiaoqing You, Chung K. Law, Combustion and Flame, 2019; 200, 15-22

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5. ISF5-Laminar Flow Reactor (Ethylene, diluted with nitrogen)
"ISF-5 main"

5.1. Reason for choosing:

a. A comprehensive data collection of gas, PAH, and soot yield in the low temperature region, 1173-1473 K, as well as individual PAH measurement.

5.2. Flame conditions:

a. Fuel: Ethylene/N2: X_{C2H4}=0.03; Inlet flow rates: 1 l/min
b. Reactor temperatures: 1173-1473 K

5.3. Available data:

a. Axial temperature profiles
b. Soot yield measurement using filter
c. Gas yield measurement using GC/MS
d. PAH yield measurement using we chemistry
e. no morphology data is available from TEM images.
f. no particle mass data is available from CPMA or APM.

5.4. References:

1. Nazly E. Sánchez, Alicia Callejas, Ángela Millera, Rafael Bilbao, and María U. Alzueta Energy & Fuels 2012 26 (8), 4823-4829 DOI: 10.1021/ef300749q

6. ISF5-Laminar Flow Reactor (Ethylene)

6.1. Reason for choosing:

a. Detailed measurements of major and minor species including PAHs up to A_2R_5 in pyrolysis condition. Excellent for mechanism validation in low temperature condition.

6.2. Flame conditions:

a. Fuel: Ethylene: X_{C2H4}=1.0; Inlet velocity: 5 cm/s
b. Reactor temperatures: 1173-1473 K
c. Reactor pressure: 8 kpa

6.3. Available data:

a. Axial temperature profiles
b. Species measurement using GC/MS
c. No soot data
d. no morphology data is available from TEM images.
e. no particle mass data is available from CPMA or APM.

6.4. References:

1. Norinaga, K., Janardhanan, V.M. and Deutschmann, O. (2008), Detailed chemical kinetic modeling of pyrolysis of ethylene, acetylene, and propylene at 1073–1373 K with a plug-flow reactor model. Int. J. Chem. Kinet., 40: 199-208. doi:10.1002/kin.20302