

Effects of ambient CO2 and H2O on soot formation in n-dodecane spray combustion $$$T_{Case=O_2=N_2}$$



CO₂ XCO₂ H₂O XH₂O

3.63

-0

0

0

15

15 85

75.15

6.22 0

0

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Approach

CFD models:

Turbulence model	LES
Primary break-up	Rosin-Rammler
Secondary break-up	Reitz-Diwakar
Collision model	No
Heat transfer	Ranz-Marshall

Chemical mechanism:

Yao mechansim: 54 species and 269 reactions

Combustion model:

Well-Stirred-Reactor (WSR)+Chemistry coordinate mapping (CCM)

Soot model: Two-equation model

$$\frac{\partial}{\partial t}(\rho Y_{soot}) + \frac{\partial}{\partial x_{j}}(\rho u_{j}Y_{soot}) = \frac{\partial}{\partial x_{j}}\left(\frac{\mu_{t}}{Sc_{t}}\frac{\partial Y_{soot}}{\partial x_{j}}\right) + \frac{dM_{soot}}{dt}$$
$$\frac{\partial}{\partial t}(\rho\phi_{N}) + \frac{\partial}{\partial x_{j}}(\rho u_{j}\phi_{N}) = \frac{\partial}{\partial x_{j}}\left(\frac{\mu_{t}}{Sc_{t}}\frac{\partial\phi_{N}}{\partial x_{j}}\right) + \frac{1}{N_{A}}\frac{dN_{soot}}{dt}$$

Numerical results

CO₂ XCO₂ H₂O XH₂O Case O₂ N₂ Thermal effects 15 75.15 6.22 0 - 0 3.6315 85 20 0 0 3 15 75.15 6.223.630 $\times 10^3$ 60 2.4 Mean flame temperature [K] Case Case 2 Case 2 50 2.2 Case 3 Case 3 Soot mass [ug] 2.0 Therma 40 effect 1.8 Chemica 30 1.6 20 .4 10 .2 --- Time-averaged(2-3.4ms 0.0 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 0 2 3 ASOI [ms] Equivalence ratio [-] 25 250 Case 2 Case 2 Case 2 Case 3 Case 3 Case 3 O radical mass [µg] 20 200 C_2H_2 mass [µg] OH mass [µg] 0.8 15 150 0.6 10 100 0.4 50 0.2 0.0 0 2 2 3 2 3 0 3 0 0 ASOI [ms] ASOI [ms] ASOI [ms]





Chemical effects

Effects of ambient H2O addition



Conclusion

(1) Thermal effects of CO2 and H2O additions promote soot formation, Chemical effects of CO2 and H2O additions suppress soot formation.

 (2) Chemical effects of CO2 addition inhibit soot formation mainly via lowering C2H2 production. This stems from the reaction: CH2*+CO2 = CH2O+O

 (3) Chemical effects of H2O addition inhibit soot formation mainly via lowering C2H2 production but enhancing OH production. The responsible reaction is: OH+H2 = H2O+H