Overpressure in the FAA Aerosol Can Test with Halon Replacements

INTERNATIONAL AIRCRAFT SYSTEMS FIRE PROTECTION WORKING GROUP MEETING

Philadelphia, PA; Dec. 3 - 5, 2013

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Kinetics	Valeri Babushok,	Flame modeling	*(NIST GR)*
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Project Goal

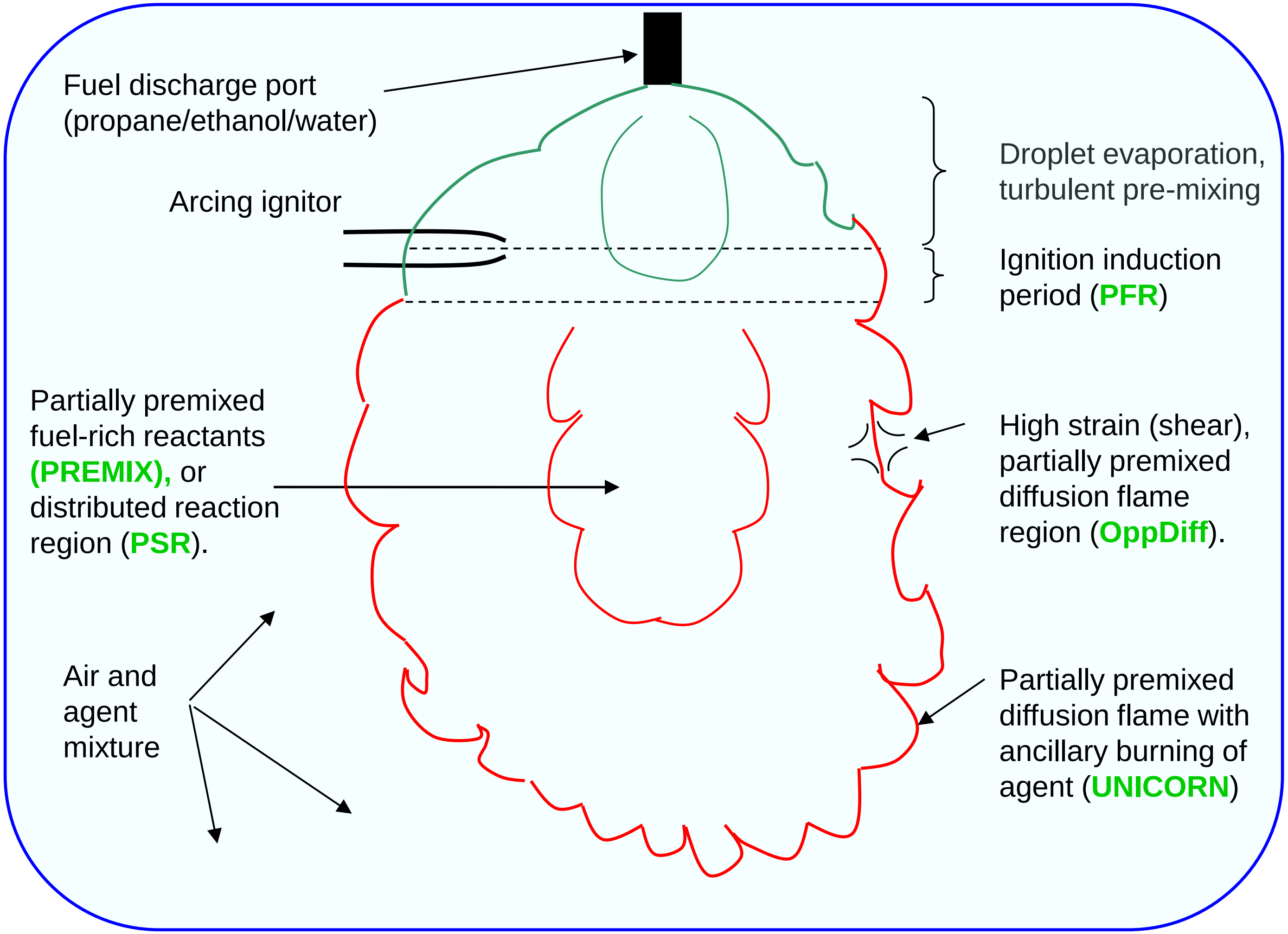
Why did overpressure occur in the Aerosol Can Test with halon replacements but not with halon 1301?

Can anything be done about it (with regard to drop-in replacements)?

Approach

Physics in FAA test is too complicated to examine with detailed kinetics, so

1. Simplify: use flame descriptions which will be accurate in some parts of the test.



Steps Taken

1. Literature Review

2. Code Assembly

3. Kinetic Mechanism Development

4. Thermodynamic Equilibrium Calculations

5. Combustion Simulations (flame modeling of: mass, momentum, and energy conservation with detailed kinetics.

6. Model validation via existing experimental data.

7. Experiment Development
   - to validate the models
   - for reduced-scale tests to investigate concepts.
   - for performing screening tests

8. Analysis of results => controlling parameters.

New Kinetic Models Were Developed*

Aerosol Can Test Kinetic Model	Species	Reactions	Type
C_3-C_4 Hydrocarbon mechanism (Wang et al.) with C_2H_50H reactions (Dryer et al.)	116	820	Acquired
NIST C_1, C_2 HFC, for hydrocarbon flame inhibition + update for pure flames	171	1467	Updated, Developed
FM200	178	1504	Updated
Novec 1230	181	1513	Developed
CF_3Br	181	1568	Updated
CF_3I	181	1563	Updated
2-BTP	188	1609	Developed
HCFC-123	242	1959	Developed

* It should be emphasized that the mechanisms adopted for the present calculations should be considered only as a starting point. Numerous changes to both the rates and the reactions incorporated may be made once a variety of experimental and theoretical data are available for testing the mechanisms.

The unexpected overpressure is due to:

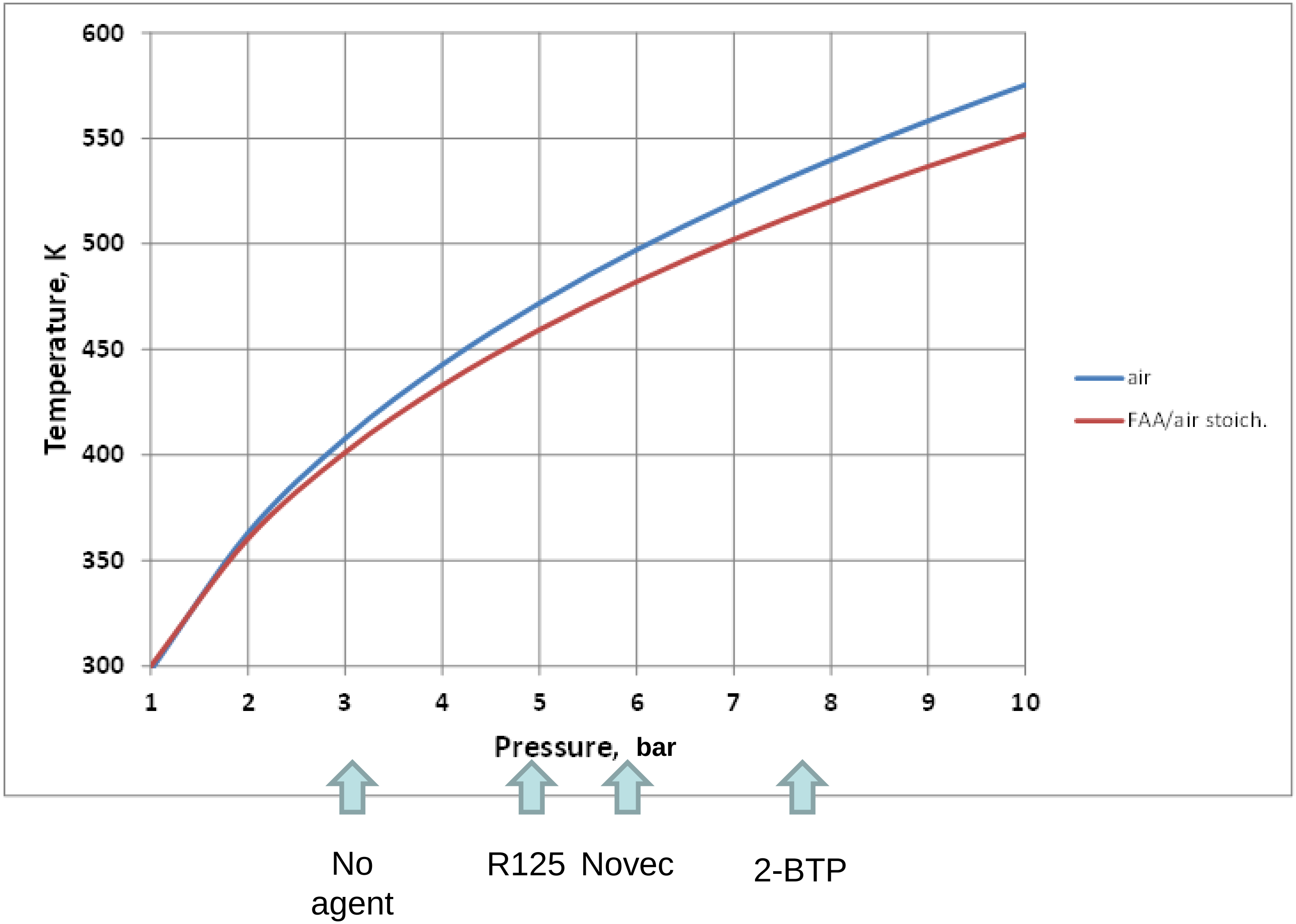
Properties of the Aerosol Can Test

1. Compressive heating
2. ≈ Match between vessel volume, fuel mass, and agent loading
3. High water content
4. Strain rate varying over chamber domain
5. Strong, continuous ignition source.
6. Lack of fire-induced vitiation.

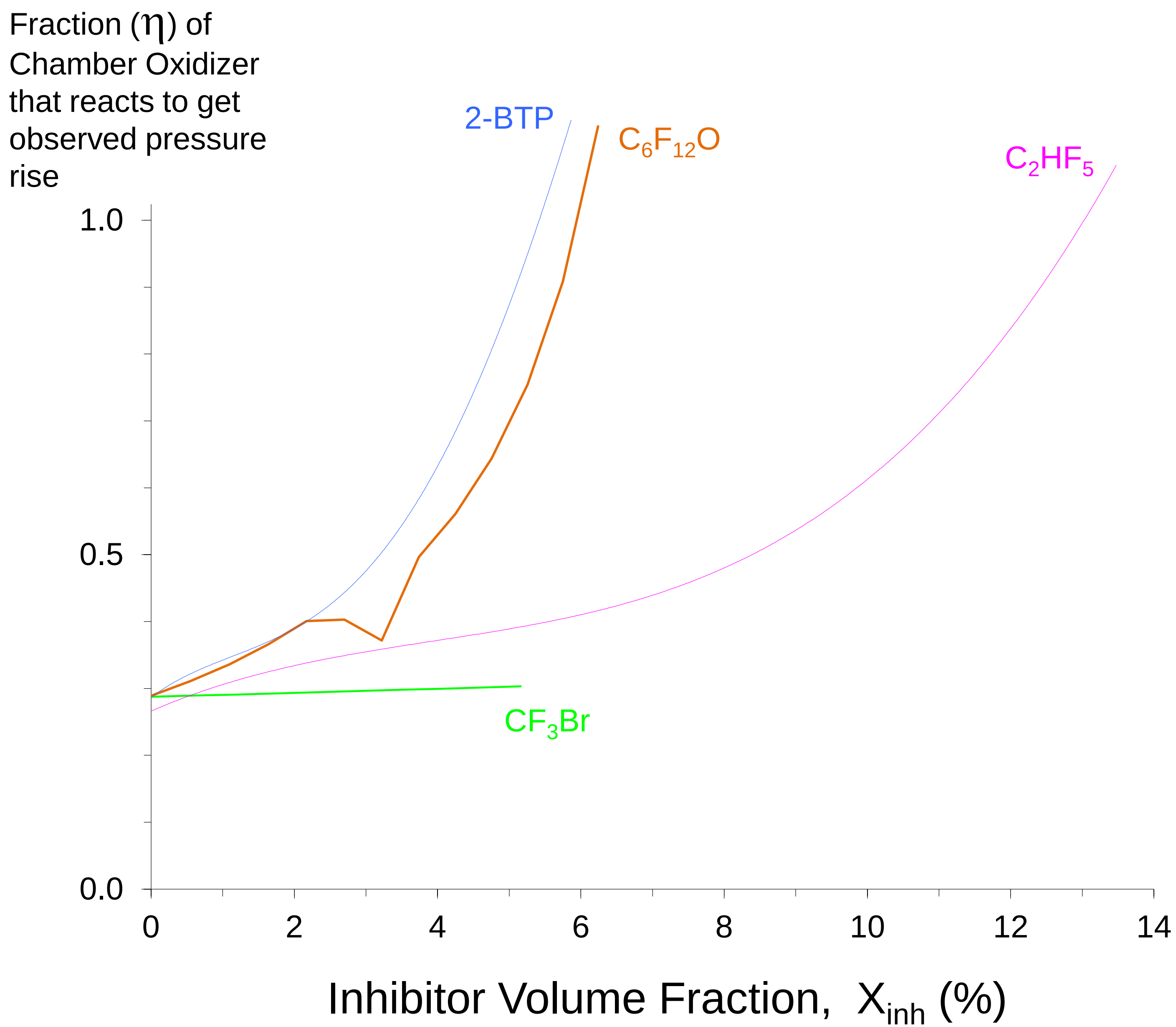
Properties of the Agent

1. Exothermic reaction
   a.) as pure compounds in pre-heated air
   b.) added to lean mixtures
   c.) in oxidizer of co-flow diffusion flame
2. Oxygen demand of agent
   a.) increases flame domain, m_{react}
   b.) varies with agent
3. Overall Reaction Rate of Agent Increases with:
   a) temperature
   b) H_2O addition
   c) higher H, C, = content in molecule.

Compressive heating increases temperature of reactants by 100 C to 200 C



≈ Match between chamber volume, fuel mass, and agent loading => high ΔP



High water content in system can enhance fluorocarbon flammability.

Compound	Moles
Fuel:	
Propane	2.05
Ethanol	5.87
Water	5.00
Oxidizer (21 ^{o}C, 100 % R.H.):	
Air	467
Water vapor in air	≤ 11.7
Agent	≤ 63

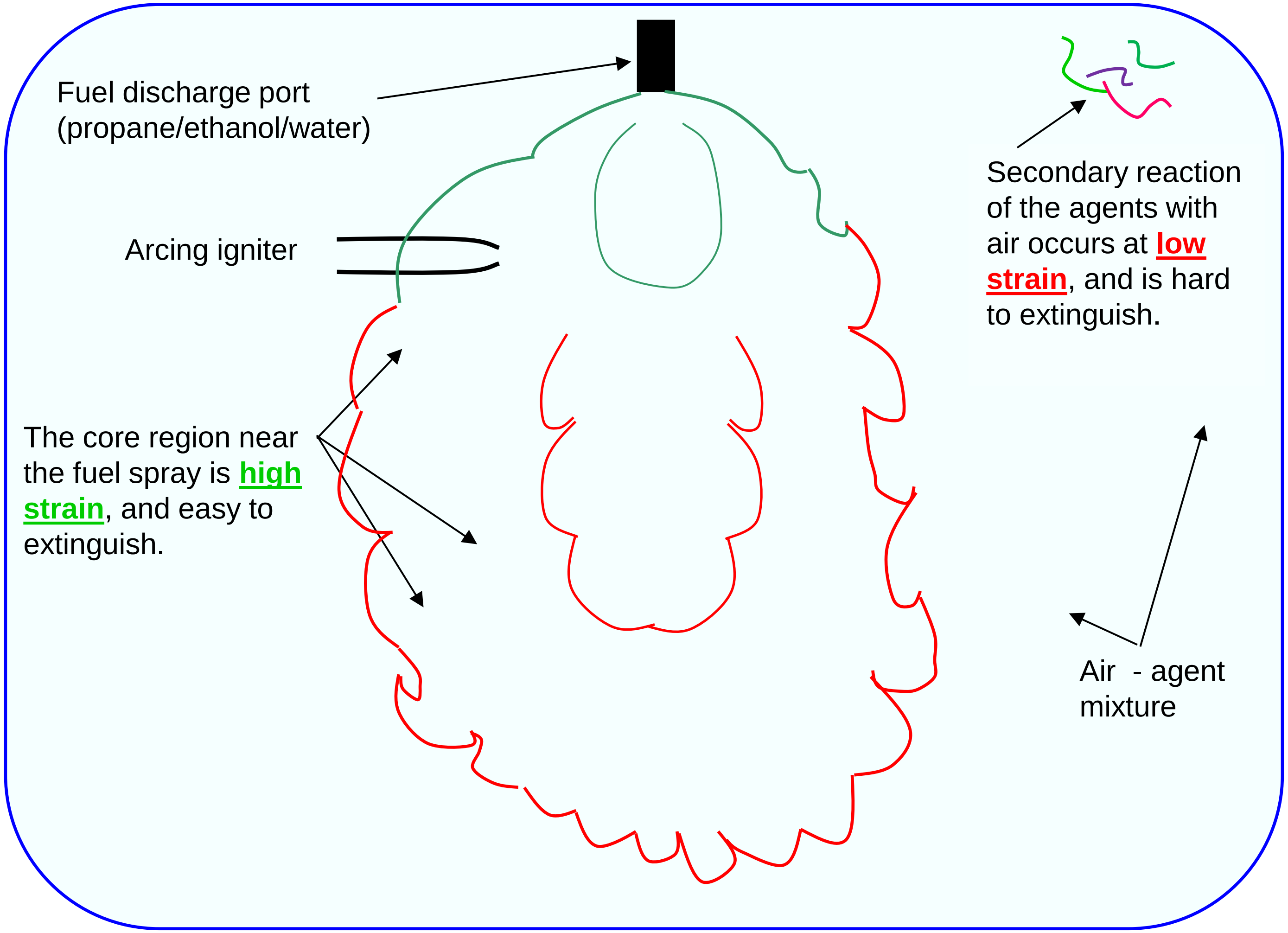
About twice as much water as fuel (@21^{o}C, 100%R.H.).

21 ^{o}C, 100 % R.H.): => X_{H2O} = 0.036

37 ^{o}C, 100 % R.H.): => X_{H2O} = 0.074

Return

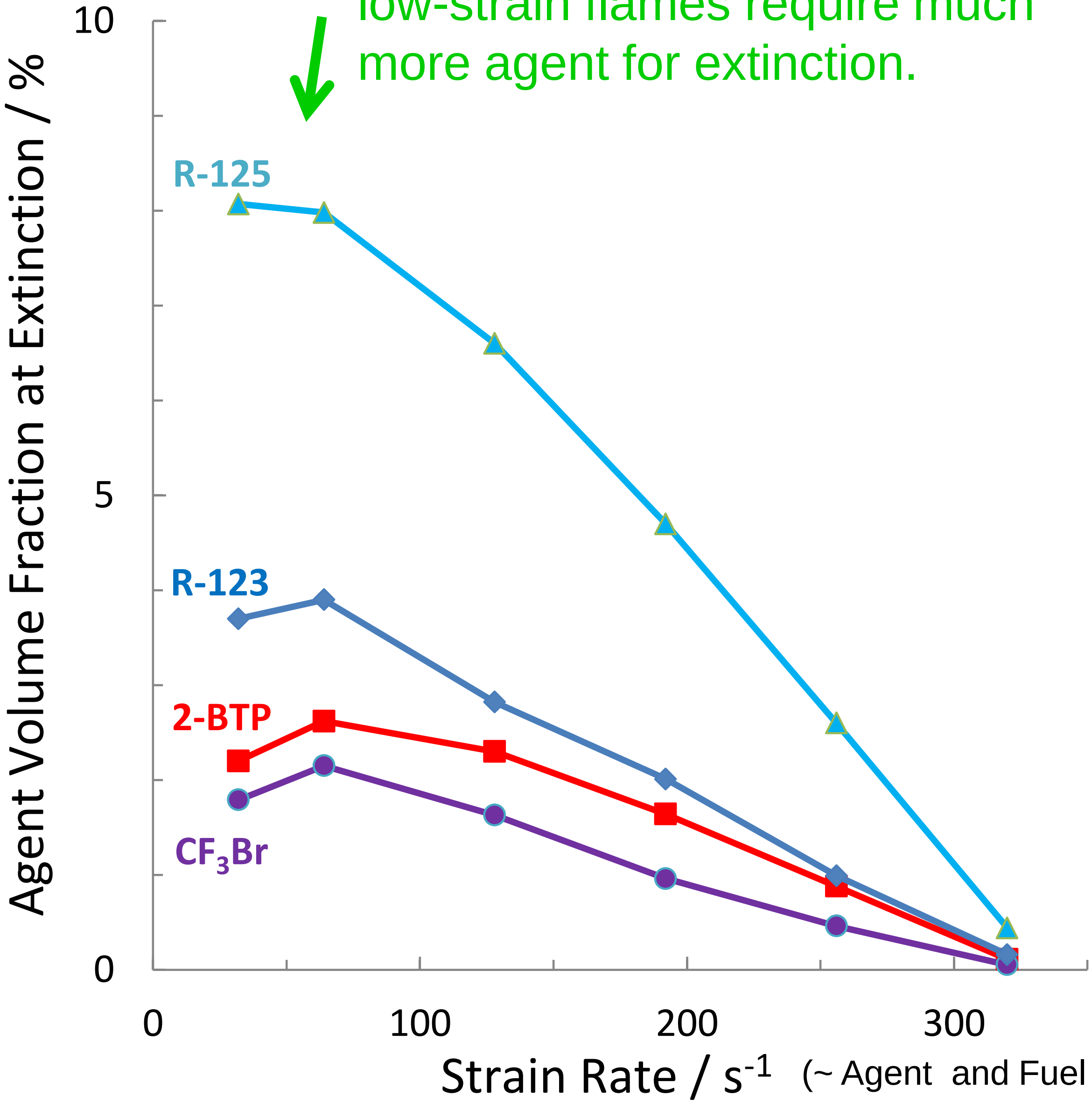
Strain rate varies over chamber domain

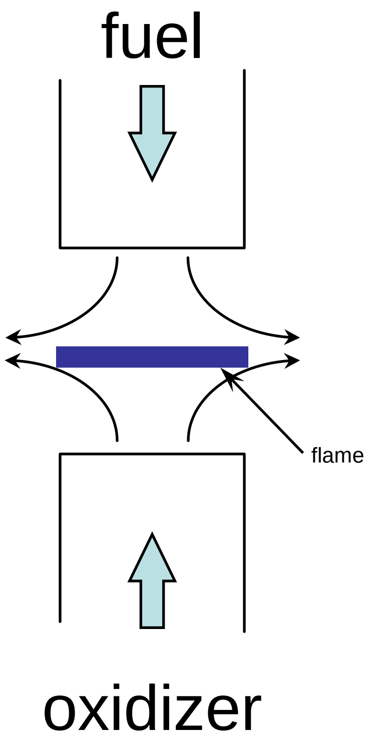


=> Adding a mildly flammable agent creates low-strain regions that are harder to extinguish

Effect of Strain Rate on Agent Extinction Concentration in Counterflow Flame

low-strain flames require much more agent for extinction.





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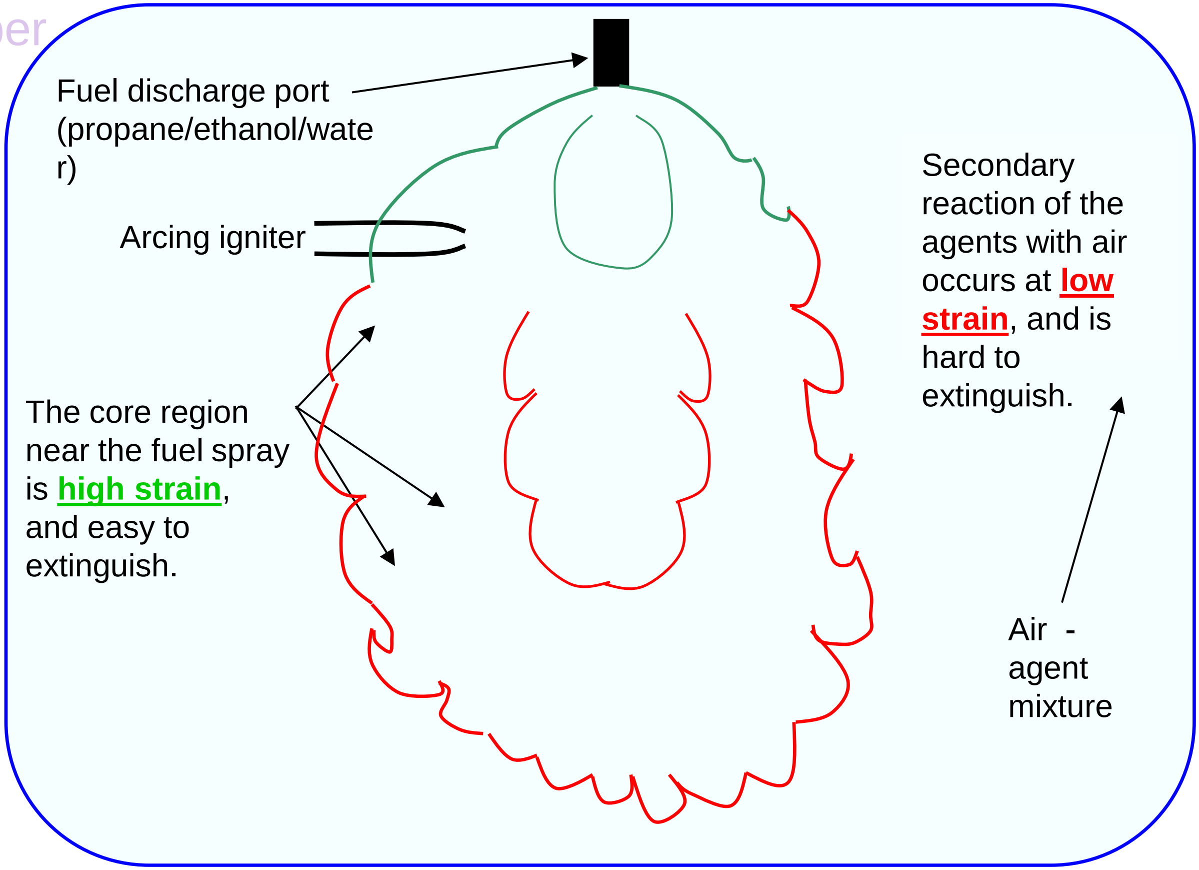

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Exothermic reaction of pure agents in air

Calculated Temperature and Burning Velocity of fire suppressant/air stoichiometric mixtures (1 bar)

(Premixed burning velocity is a measure of the mixture's overall reaction rate.)

Agent	Formula	Oxidizer	Initial Temperature, K	Peak Adiabatic Flame Temperature K	Burning Velocity, cm/s
HFC-23	CF_3H	air	400	1751	0.567
HFC-125	C_2F_5H	air	400	1858	1.56
HFC-227ea	C_3F_7H	air	400	1874	2.48
2-BTP	$C_3H_2F_3Br$	air	400	2033	2.14
Novec 1230	$C_3F_7COC_2F_5$	air	400	1864	0.367
Triodide	CF_3I	oxygen	500	1528	1.33
halon-1301	CF_3Br	oxygen	500	1485	<0.15

(values down to ≈1 cm/s can be measured.)

- some fire suppressants themselves may support flames (although very weak) in air at elevated temperatures.

- burning velocity of CF_3Br is < 0.15 cm/s at 500 K with O_2 oxidizer.

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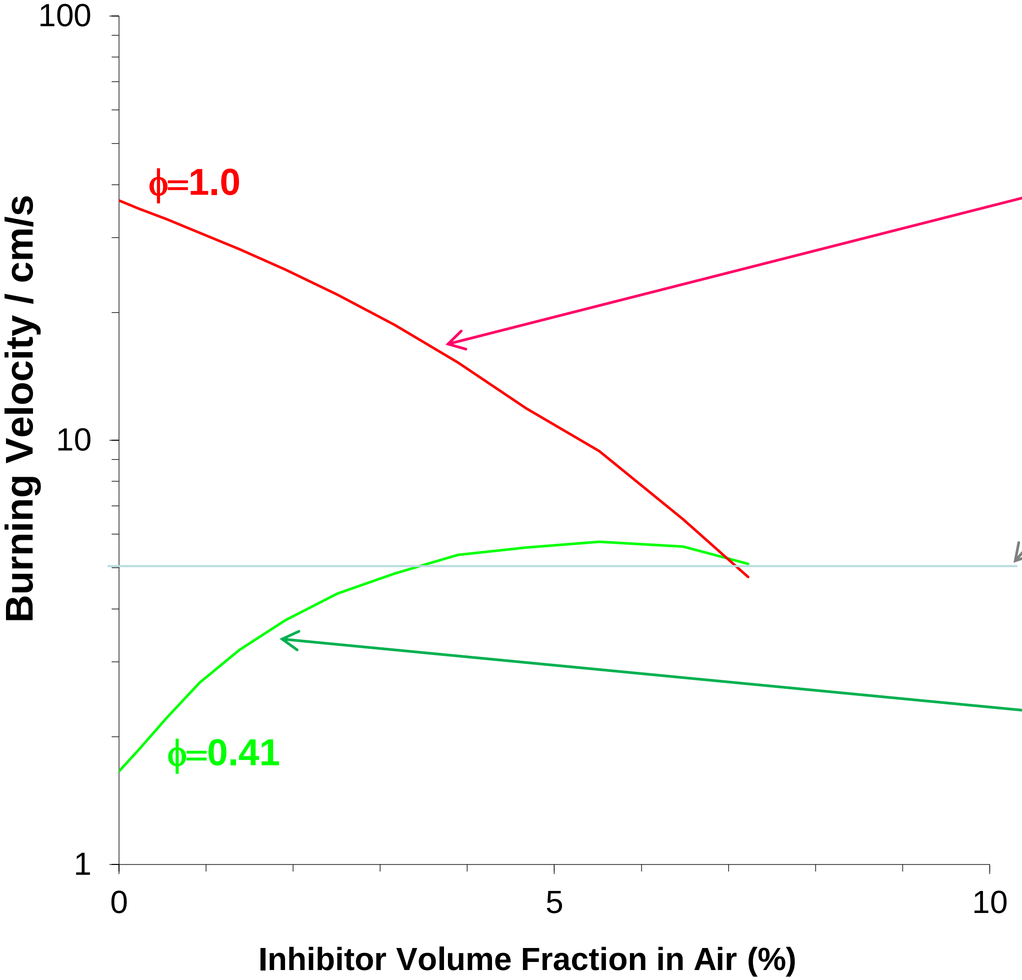
Enhanced flammability of lean flames with agent addition: HFC-125

HFC-125 with Aerosol Can Test Fuel, T_{init}=298 K



Adding suppressant to a stoichiometric flame slows the burning velocity.

A burning velocity of 5 cm/s is sometimes considered a criterion for the flammability limit.

Adding suppressant to a lean mixture can:

- increase the burning velocity, and
- bring the mixture into a flammable regime.

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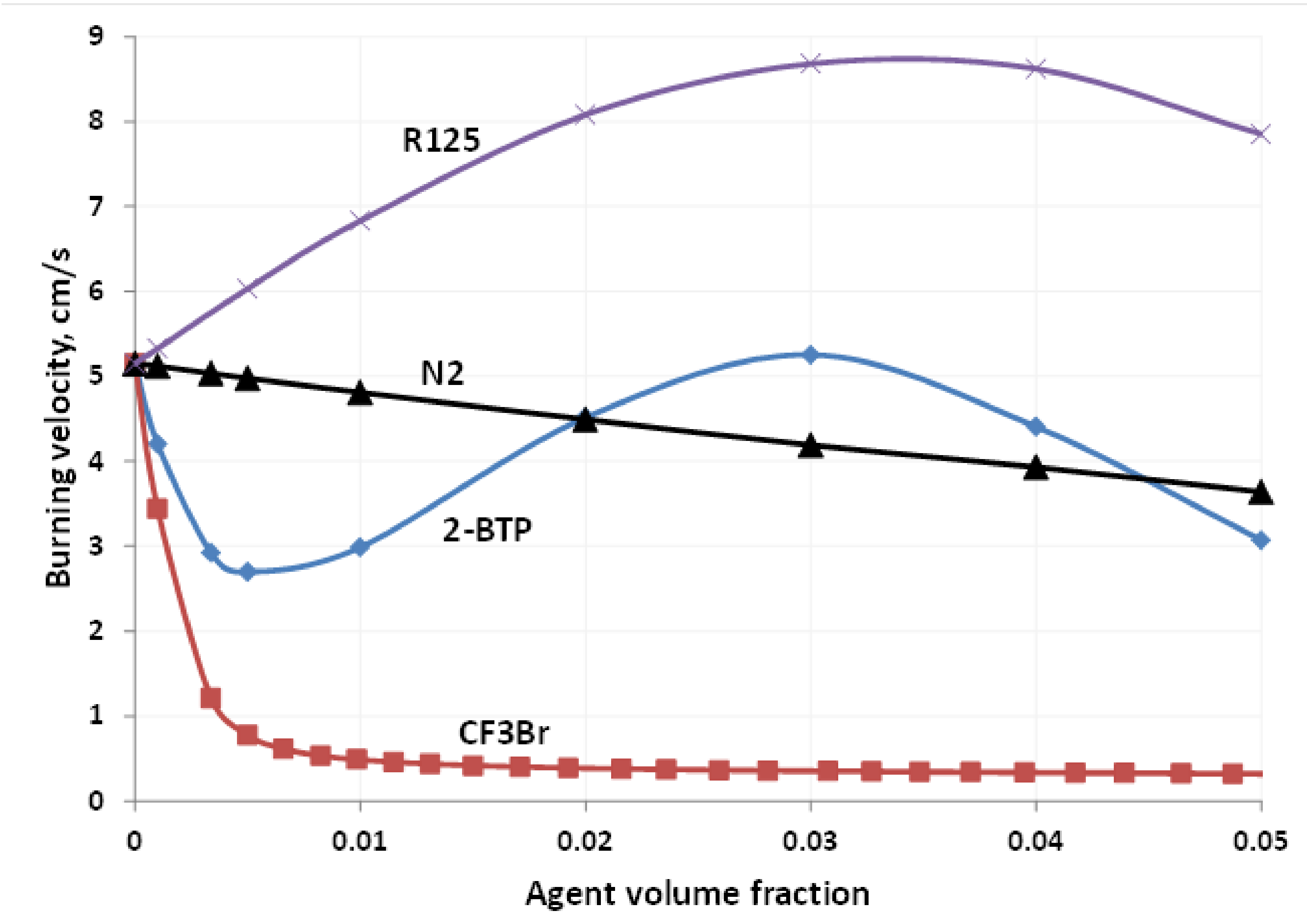
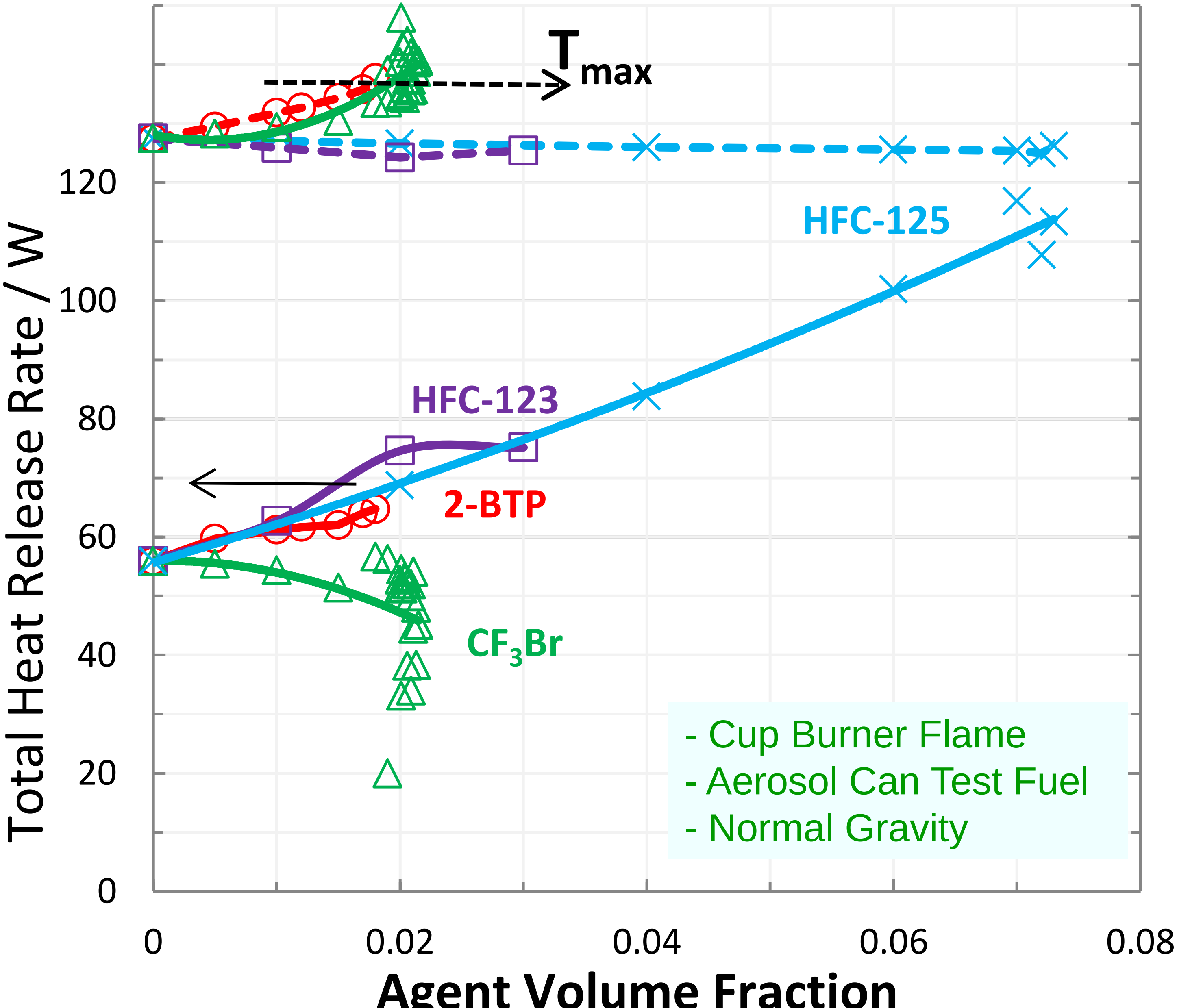
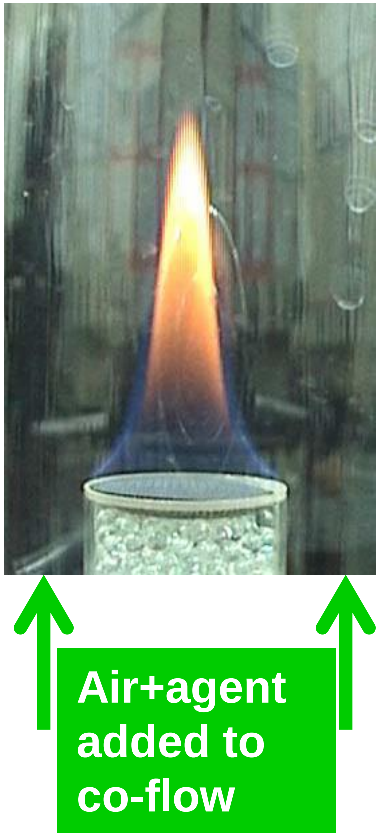
Effect of suppressant on lean flames (CH_4-air, ϕ=0.5) varies with the agent type



turn

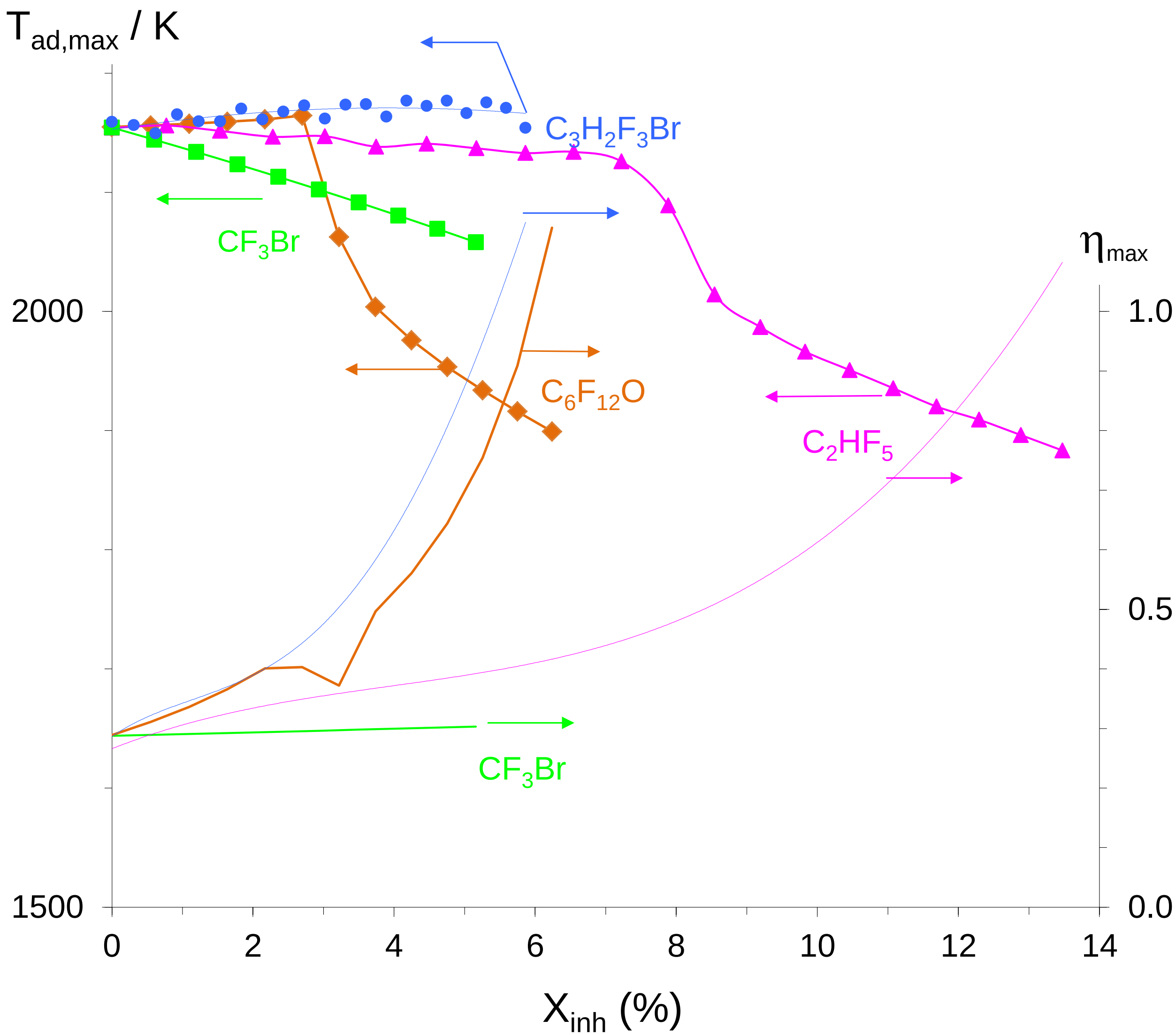
Effect of agent addition on heat release rate and peak T in cup burner



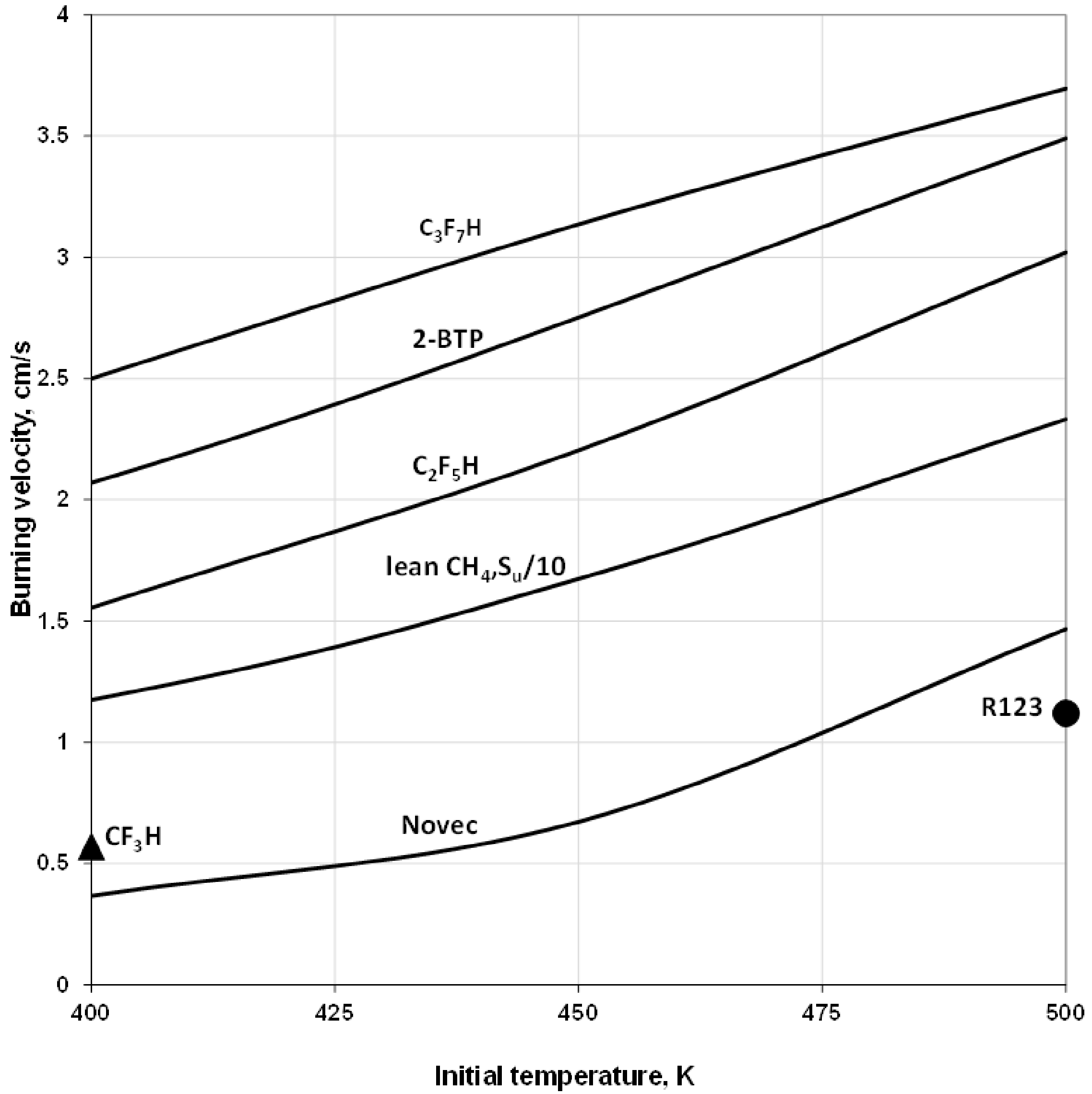


Oxygen demand depends upon agent molecule and extinction concentration

(FAA Aerosol Can Test, Calculated T_{ad} and Fraction of Chamber Volume Reacting, η)



Temperature Sensitivity of Pure Agent Burning Velocity



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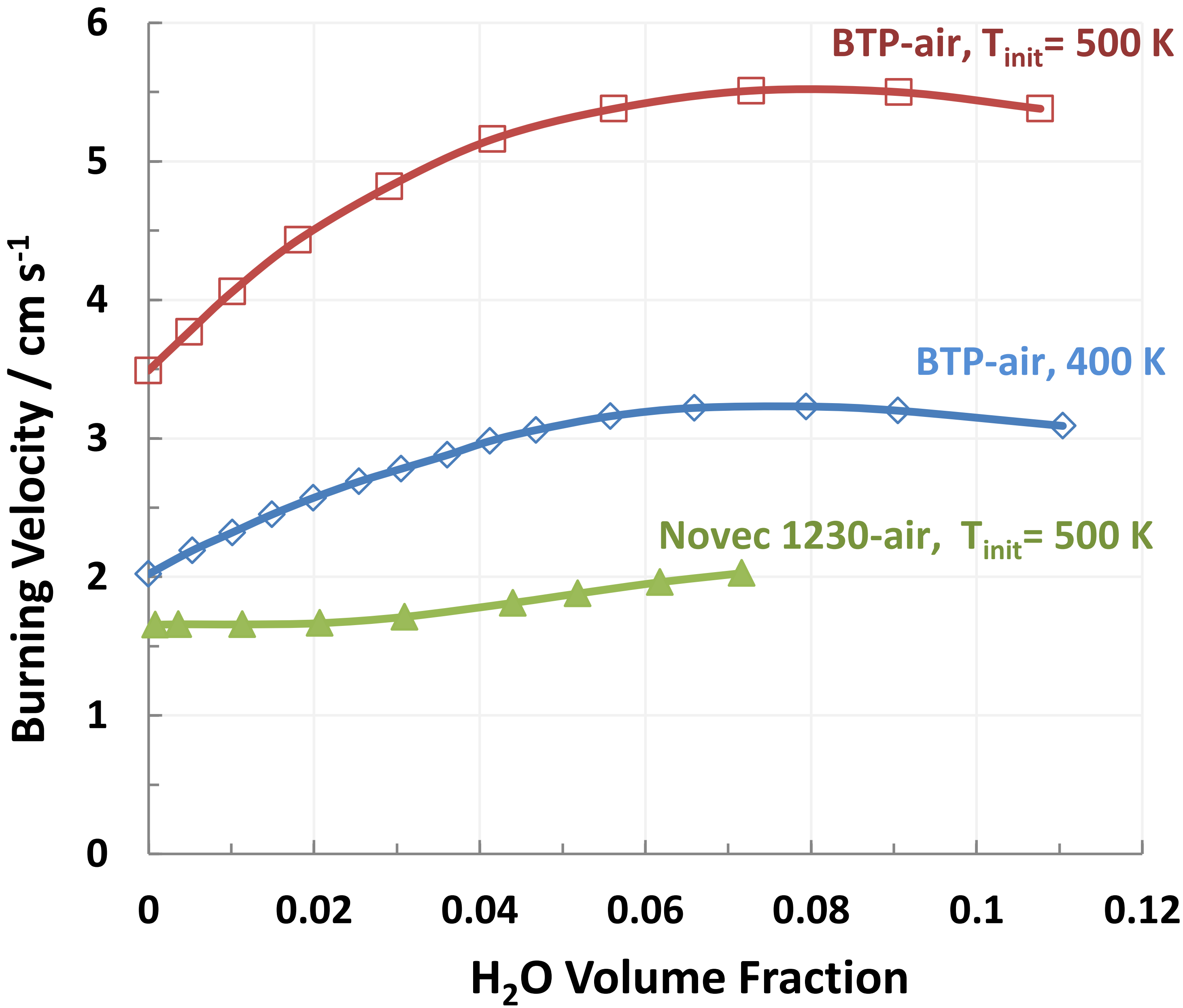
Effect of water vapor on calculated stoichiometric agent-air burning velocity



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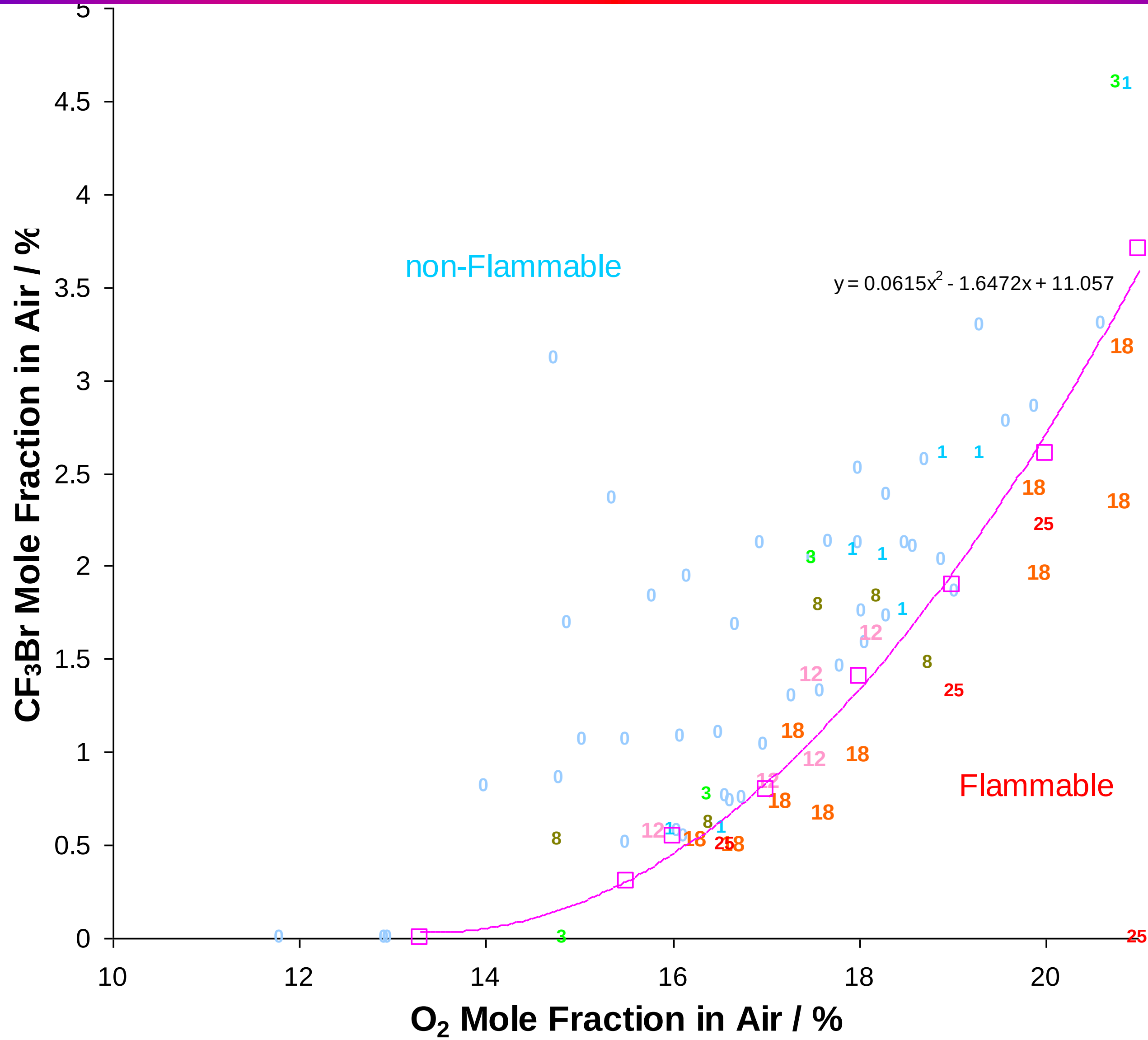
FAA-ACT with CF_3Br with Varying $X_{O2,ox}$



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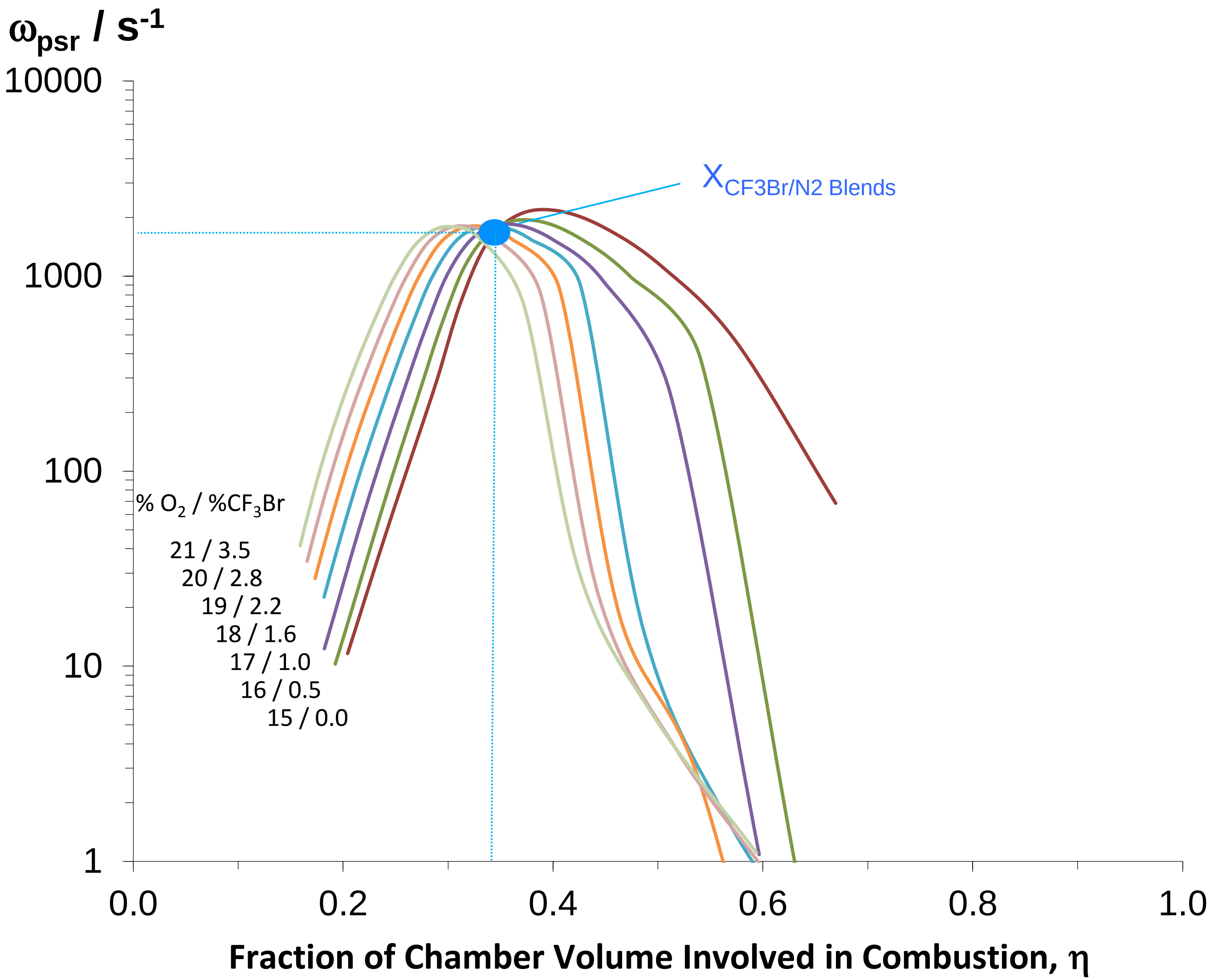
Mixtures of CF_3Br and N_2 all imply about the same value of η and ω_{psr}



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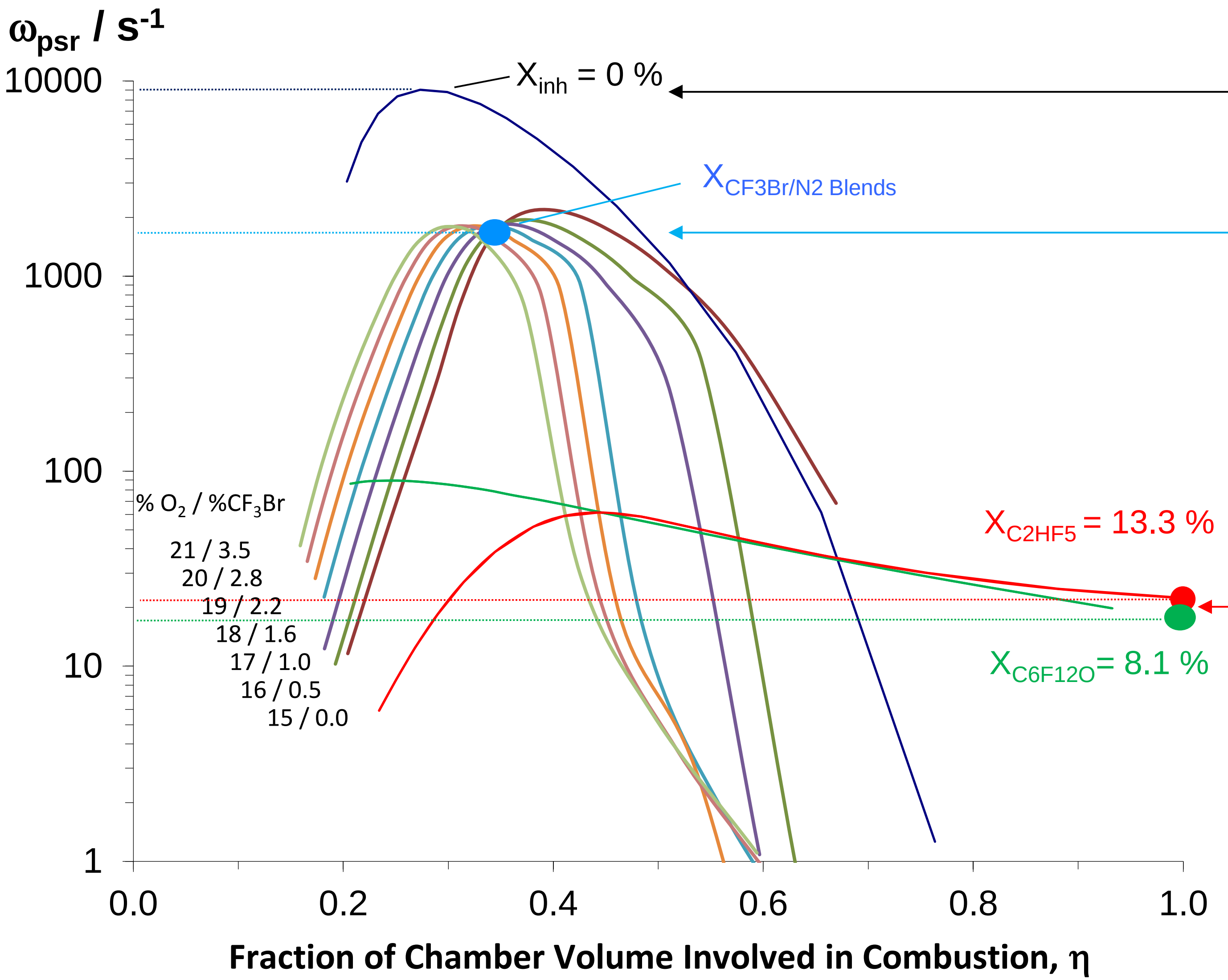
For inertion of the FAA-ACT, HFC-125, 2-BTP, or Novec 1230 must lower the reaction rate 100 x more than CF_3Br/N_2 mixtures



Uninhibited flames have a reaction rate of about 9000 s^{-1}.

CF_3Br / N_2 Mixtures Show that in Turbulent Zone, the overall reaction rate must be lowered below about 1800 s^{-1} for inerting (i.e., lower rxn rate by 5x)

Whereas with added R125, Novec, or 2-BTP, the overall reaction rate must be lowered to about 20 s^{-1} for FAA-ACT extinction (i.e., 100x lower reaction rate than in the turbulent zone).

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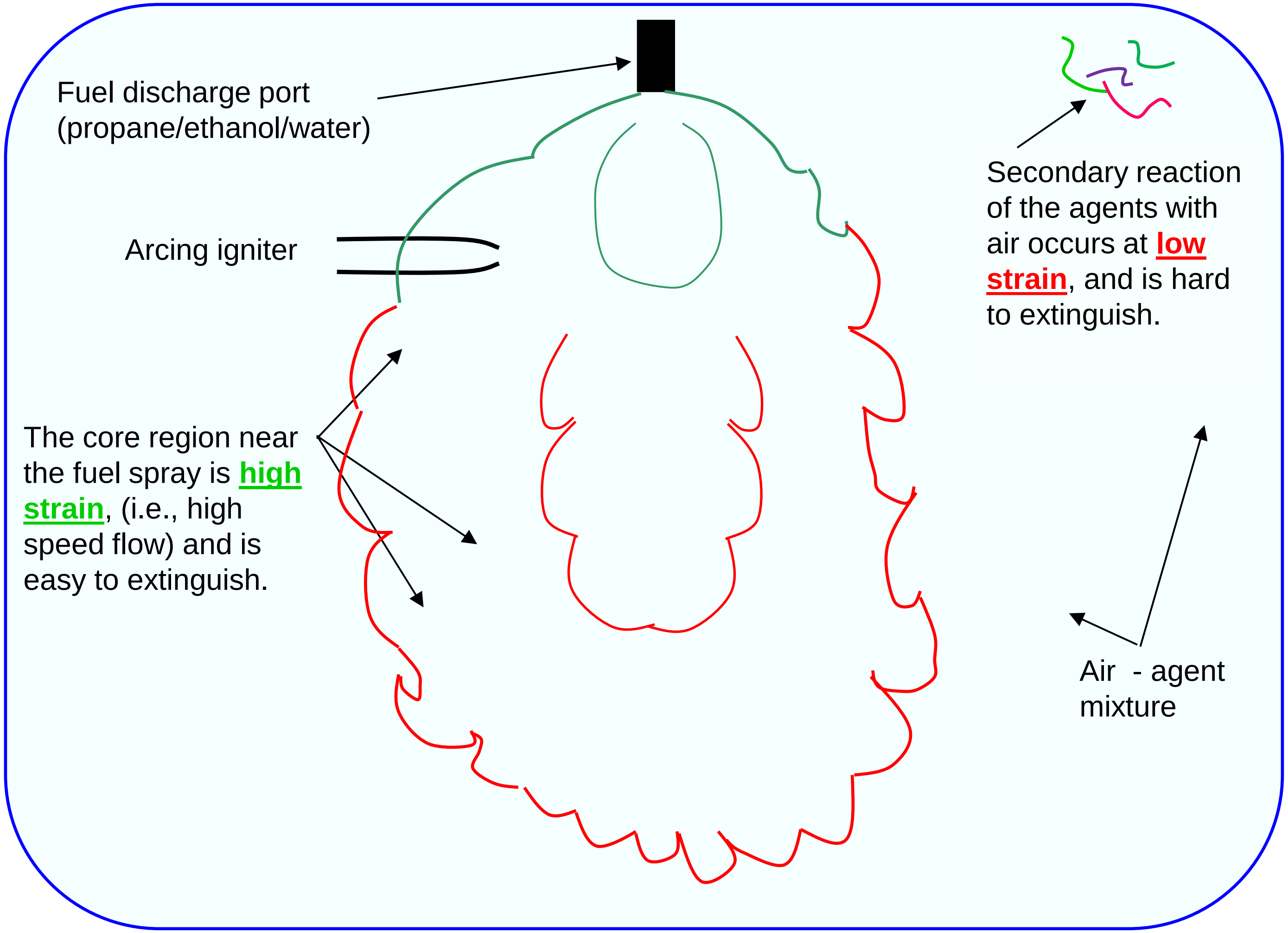
Strain rate varyies over chamber domain



=> Adding a mildly flammable agent creates low-strain regions that are harder to extinguish

Possible Solutions

1. Blends:

All of the tested (and obvious) agents (R-125, 2-BTP, Novec, CF3I, R123) with and inert, with each other, etc.

2. New Agent:

- less HC char (C, H, double bonds), more chemically active species: I, Cl, Br, P, etc.;
- R123, R123-like;
- 2-BTP with H replaced by F, Cl, Br, etc.
- look at whole universe of possibilities again.

3. Completely New Approach:

- Water mist + N2.
- Inert gas generator with higher boiling point agent?

Next Steps/Future work

1. Experimentally Validate Mechanisms (for $C_3BrF_3H_2$, R123, Novec, CF_3I) then run calculations for:
   a.) Mixtures
   b.) Varying $X_{O2,ox}$.
   c.) New agents (BTP with H replaced by F, Br, Cl, etc.)
2. Perform experiments in reduced-scale tests with candidate agents (e.g., BTP-2Br, BTP-Cl BTP-F, etc).
3. Perform new tests at the FAA ACT facility to test concepts, and try combinations:
   a.) R123; R123 as $f(X_{O2,ox})$
   b.) HFCO-1233 ($C_3H_2ClF_3$) as $f(X_{O2,ox})$
   c.) CF_3I; CF_3I as $f(X_{O2,ox})$
   d.) Novec as $f(X_{O2,ox})$
   e.) HFCs, HFOs, etc., with Br_2
   f.) C_2H_6 in end gas, with: no agent; CF_3Br at 2%
   g.) less fuel in aerosol can
4. Evaluate/test proposed new agents from chemical companies.
5. Develop/evaluate other, non-drop-in approaches.

Publications

1. Linteris, G.T., Takahashi, F., Katta, V.R., Chelliah, H.K., Meier, O. “Thermodynamic analysis of suppressant-enhanced overpressure in the FAA Aerosol Can Simulator,” accepted for publication in *Fire Safety Science: Proceedings of the Tenth International Symposium,* International Association for Fire Safety Science (IAFSS), Boston, MA, 2011.

2. Linteris, G.T., Takahashi, F., Katta, V.R., Chelliah, H.K., Meier, O., “Stirred Reactor Calculations to Understand Unwanted Combustion Enhancement by Potential Halon Replacements,” *Combustion and Flame*, **159**:1016-1025, 2012.

3. Babushok, V.I., Linteris, G.T., Meier, O., “Combustion Properties of Halogenated Fire Suppressants,” *Combustion and Flame*, 159(12), 3569–3575, 2012.

4. Linteris, G.T., Babushok, V.I., Sunderland, P.B., Takahashi, F., Katta, V.R.,Meier, O., “Unwanted Combustion Enhancement by $C_6F_{12}O$ Fire Suppressant,” *Proceedings of the Combustion Institute*, 34, 2683-2690, 2013.

5. Takahashi, F., Katta, V.R., Linteris, G.T., Meier, O., “Cup-burner Flame Structure and Extinguishment by CF_3Br and C_2HF_5 in Microgravity,” *Proceedings of the Combustion Institute*, 34, 2707-2717, 2013.

6. Linteris, G.T., Babushok, Takahashi, F., Katta, “The Exothermic Reaction of Fire Suppressants,” *Proc. of the Seventh International Seminar on Fire & Explosion Hazards (ISFEH7)*, pp. 443-452, Edited by D. Bradley, G. Makhviladze, V. Molkov, P. Sunderland, and F. Tamanini Copyright □ 2013 University of Maryland. Published by Research Publishing ISBN: 978-981-08-7724-8: doi: 10.3850/978-981-08-7724-8_0x-0x.

7. Babushok, V.I., Linteris, G.T., Meier, O., Pagliaro, J.L., “Flame Inhibition by CF_3CHCl_2 (HCFC-123), submitted for publication in *Combustion Science and Technology*, Aug. 2013.

8. Babushok, V.I., Burgess, D.R., Linteris, G.T., Meier, O.C. “Flame Inhibition by Bromotrifluoropropane (2-BTP) ,“ to be submitted to *Combustion and Flame*, Nov. 2013.*

9. Burgess, D.R. “Thermochemical data for the decomposition of 2-bromotrifluoropropene” to be submitted to the *Journal of Physical Chemistry A*, Dec. 2013.*

10. Pagliaro, J.L., Babushok, V.I., Linteris, G.T. and Sunderland, P.B. “Premixed Flame Inhibition by 2-BTP and HCFC-123,” to be submitted to *Combustion and Flame*, Dec. 2013.*

11. Linteris, G.T., Babushok, V.I., Takahashi, F., Katta, V.R., “Understanding Unwanted Combustion Enhancement by $C_3H_2F_3Br$ Fire Suppressant,” to be submitted to the *Proceedings of the Combustion Institute*, 2013.*

* In preparation.