NATIONAL INSTITUTE OF STANDARDS AND TECHNOLOGY
U.S. DEPARTMENT OF COMMERCE

Progress in Modeling Cup Burner Flame Extinction by Sodium Bicarbonate Powder in FDS

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Outline

- Background and motivation
- $NaHCO_3$ decomposition
- FDS model formulation
- Results
- Conclusions

Background and Motivation

D. Ingerson. Full-scale Demonstration Testing with a Solid Aerosol Fire Extinguishing Agent. FAA Nov 2012

Background and Motivation

EVALUATION OF
ALTERNATIVE IN-FLIGHT
FIRE SUPPRESSANTS
FOR
FULL-SCALE TESTING
IN SIMULATED
AIRCRAFT ENGINE
NACELLES
AND DRY BAYS

WILLIAM L. GROSSHANDLER,
RICHARD G. GANN AND
WILLIAM M. PITTS, EDITORS

NIST

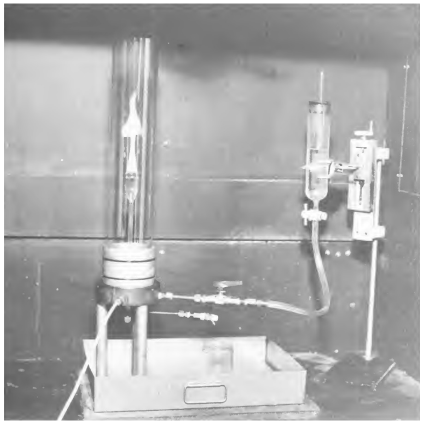
United States Department
of Commerce

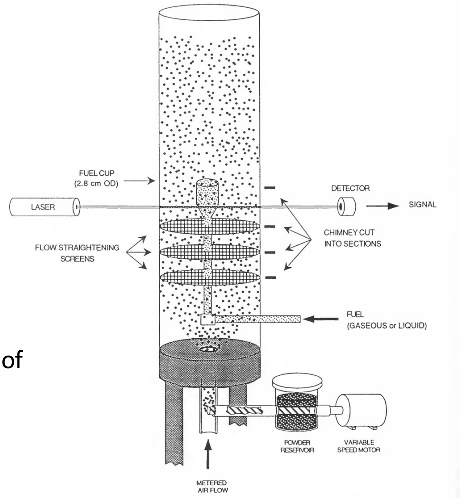
Technology Administration

National Institute of
Standards and Technology

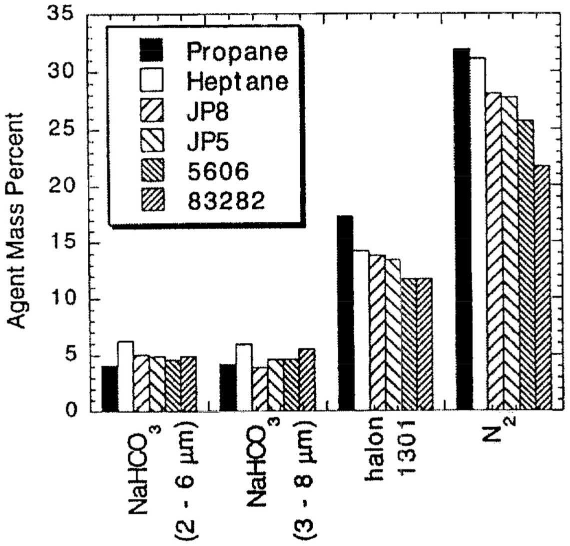
April 1994
NIST SP 861

A. Hamins, Flame Suppression Effectiveness: Coflowing Non-premixed Flames, in: W. L. Grosshandler, R. G. Gann, W. M. Pitts (Eds.), Evaluation of Alternative In-Flight Fire Suppressants for Full-Scale Testing in Simulated Aircraft Engine Nacelles and Dry Bays, NIST SP 861, chap. 4.3, Gaithersburg, Maryland, 377–400, 1994.





"A comparison of agents showed that on average, **NaHCO3 was three times more effective than CF3Br on a mass basis and six times more effective than N2** in extinguishing flames burning the various fuels."



Previous Work

- **A. Hamins, Flame Suppression Effectiveness: Coflowing Non-premixed Flames**, in: W. L. Grosshandler, R. G. Gann, W. M. Pitts (Eds.), Evaluation of Alternative In-Flight Fire Suppressants for Full-Scale Testing in Simulated Aircraft Engine Nacelles and Dry Bays, NIST SP 861, chap. 4.3, Gaithersburg, Maryland, 377–400, 1994.
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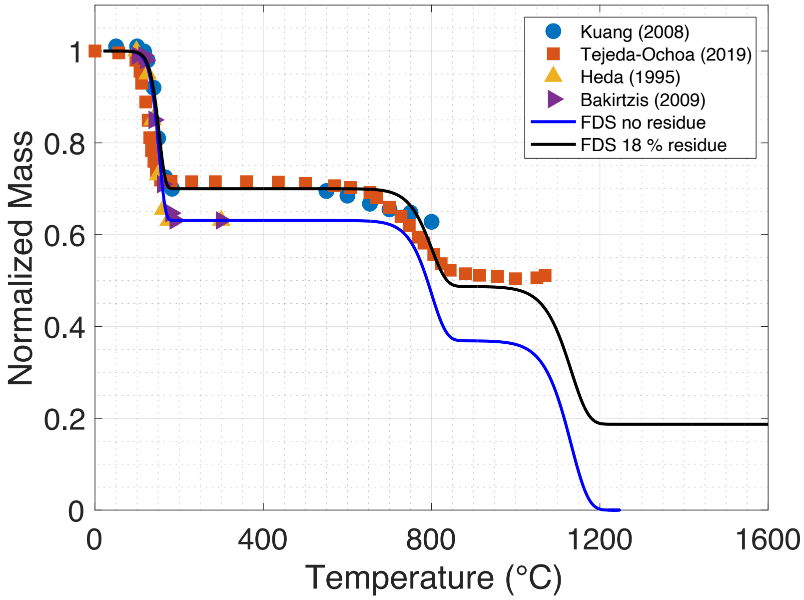
- H. K. Chelliah, P. C. Wanigarathne, A. M. Lentati, R. H. Krauss, G. S. Fallon. Effect of sodium bicarbonate particle size on the extinction condition of non-premixed counterflow flames. Combust. Flame 134 (2003) 261–272.
- O. Dounia, O. Vermorel, T. Poinsot, Theoretical analysis and simulation of methane/air flame inhibition by sodium bicarbonate particles, Combust. Flame 193 (2018) 313–326.

$NaHCO_3$ Decomposition Kinetics

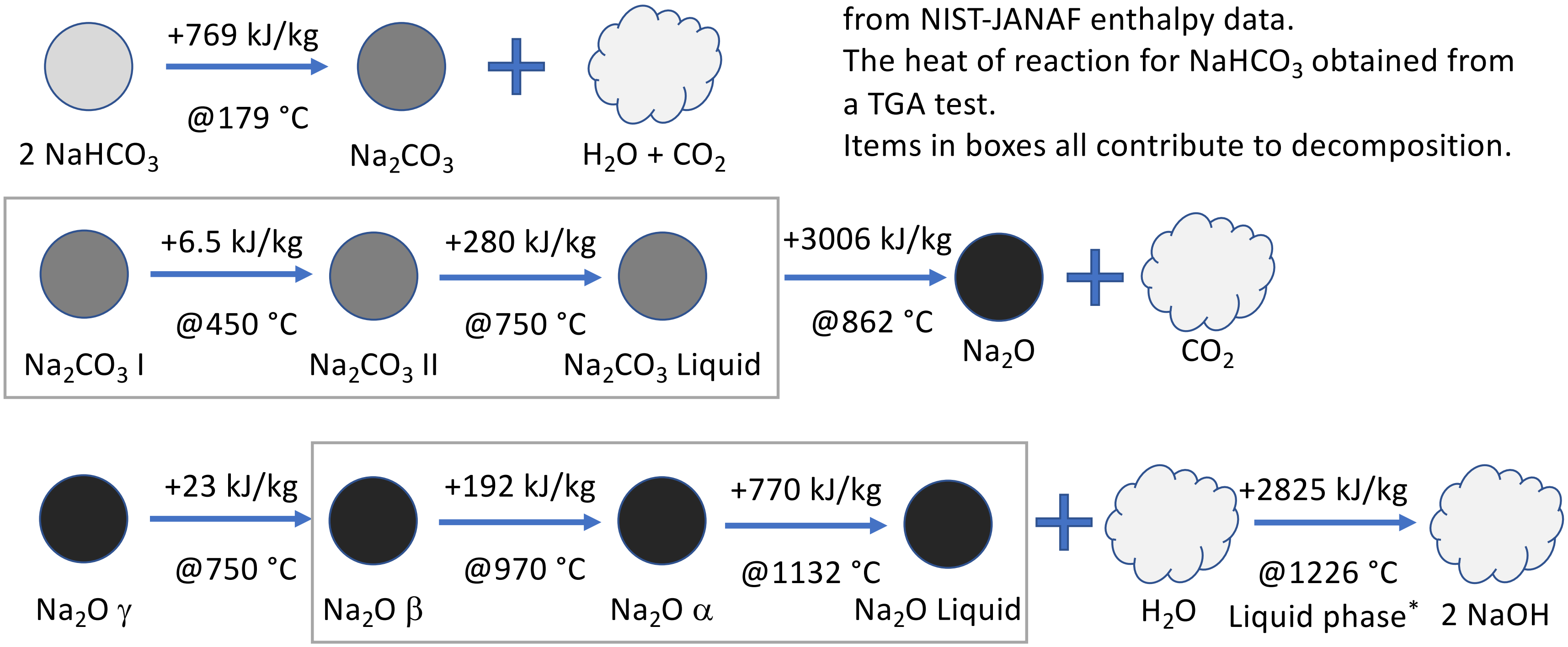
Reaction	Temp [°C]	E_a [kJ/mol]	A [1/s]
$NaHCO_3$ (s) $\rightarrow \frac{1}{2}Na_2CO_3$ (s) $+ \frac{1}{2}CO_2 + \frac{1}{2}H_2O$	98.4 - 168	105.8	1.1×10^{11}
Na_2CO_3 (s) $\rightarrow Na_2O$ (s) $+ CO_2$	550 - 900	273.3	9.5×10^{10}
Na_2O (s) $+ H_2O \rightarrow 2\,NaOH$	900 - 1200	401.6	3.4×10^{12}



- TGA at 10 K/min
- Mass loss on heating process of $NaHCO_3$ is divided into three stages.
- The mass loss in first and second stages are validated with available literature data of pure $NaHCO_3$ at low temperature of 98 - 168 °C and BC powder as well at $NaHCO_3$ and SiO_2 mixture at temperature of 550 - 900 °C .
- At high temperature, calculations of equilibrium concentrations demonstrate that the main product above 974 to 1127 °C is sodium hydroxide [Zamansky, 1997], homogeneous reaction $Na_2O + H_2O => 2NaOH$ is defined in temperature range of 900 - 1200 °C.
- Third step is not well understood. (We will return to this.)

NaHCO3 Decomposition Thermodynamics

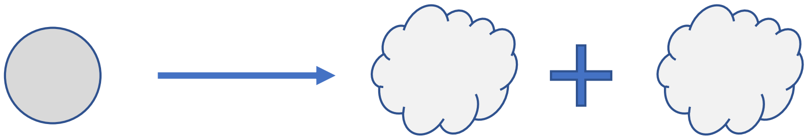
Heats of reaction for $NaCO_3$ and Na_2O obtained from NIST-JANAF enthalpy data.
The heat of reaction for $NaHCO_3$ obtained from a TGA test.
Items in boxes all contribute to decomposition.



Not well understood, we follow Dounia (2018)

* β and α phases would differ by the phase change energy

Simplified Full Particle Decomposition

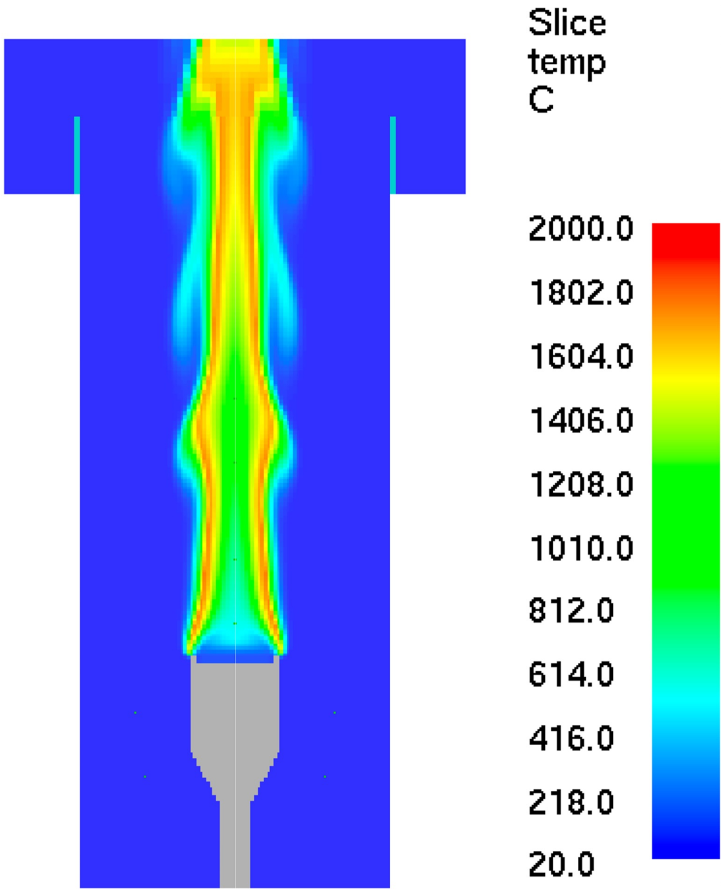


1 kmol $NaHCO_3$	1 kmol CO_2	1 kmol NaOH
1 kg $NaHCO_3$	0.524 kg CO_2	0.476 NaOH

“The residence time in the cup burner flames used here is approximately an order of magnitude larger than in the low-strain-rate counterflow flames [used by Trees and Seshadri], suggesting that both [2 to 6 μm and 3 to 8 μm] **particle fractions completely vaporized** in the cup burner flame.” -- A. Hamins (1998)

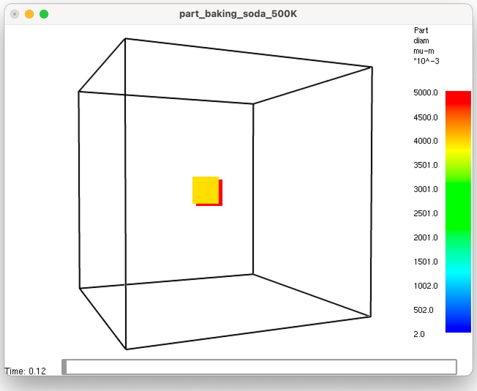
This observation will be useful for later analysis.

FDS Model Formulation



- low-Mach, 2D axisymmetric, DNS or “LES”
- generalized lumped species
- conservative, finite-volume, second-order
- TVD scalar transport (CHARM)
- modified Deardorff eddy-viscosity, algebraic k_sgs (minimal)
- constant Sc_t and Pr_t (0.5)
- gray gas radiation
- predicted radiant emission
- JANAF + NASA thermodynamic properties
- basic EDC (or EDM) combustion model
- specified threshold (AIT) ignition model
- thermal extinction model based on critical flame temperature
- solid particle thermal decomposition (new for moving particles)

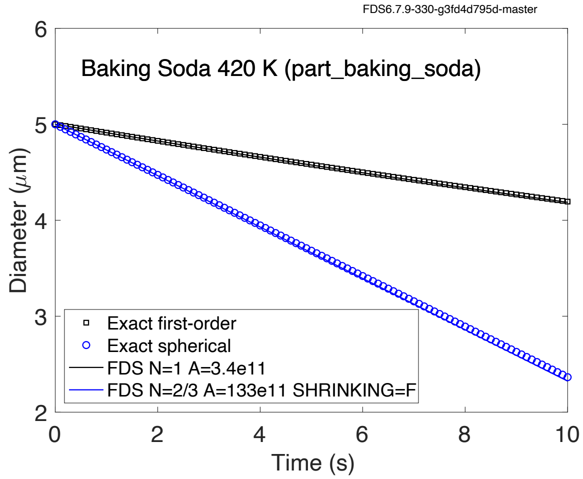
Solid particle decomposition verification

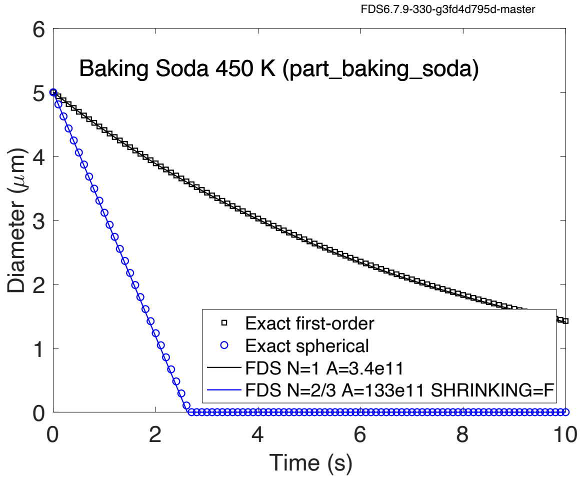


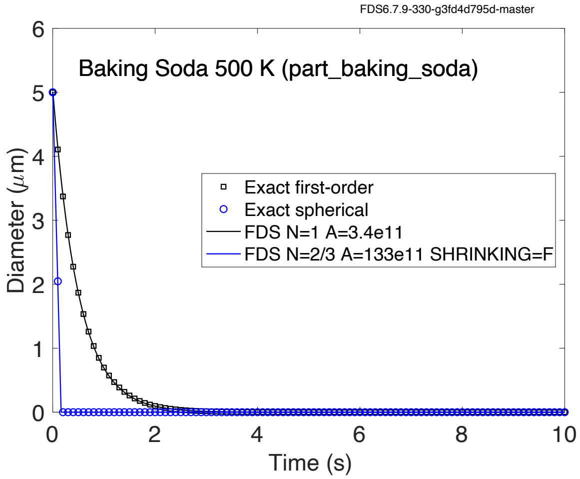
- Specified initial temperature
- SOLID_PHASE_ONLY=True
- Heat of reaction = 0 kJ/kg
- Kinetics models from Heda et al. (1995)

extent of reaction: $\alpha = \dfrac{m_0 - m}{m_0}$

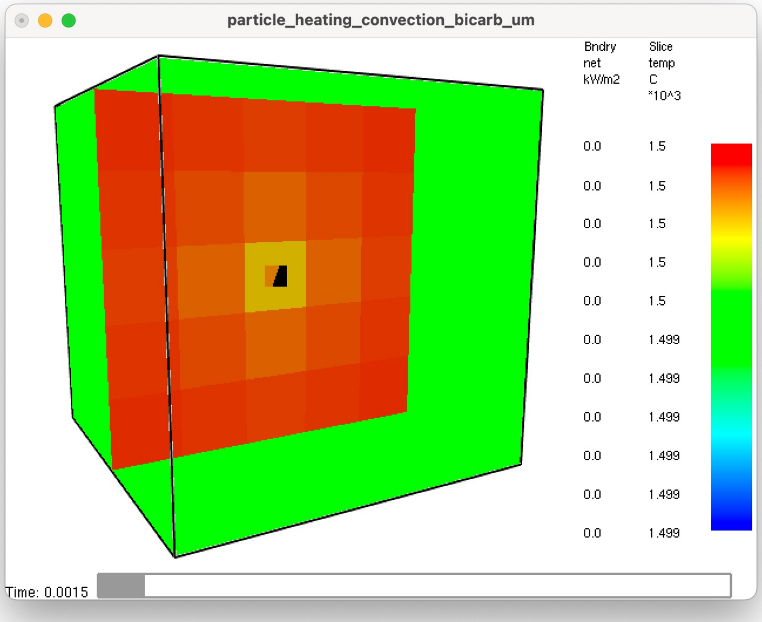
First-order	Spherical contraction
$\dfrac{\mathrm{d}\alpha}{\mathrm{d}t} = k(1-\alpha)$	$\dfrac{\mathrm{d}\alpha}{\mathrm{d}t} = k\,3(1-\alpha)^{2/3}$
$r^3 = r_0^3\,e^{-kt}$	$r = r_0(1-kt)$

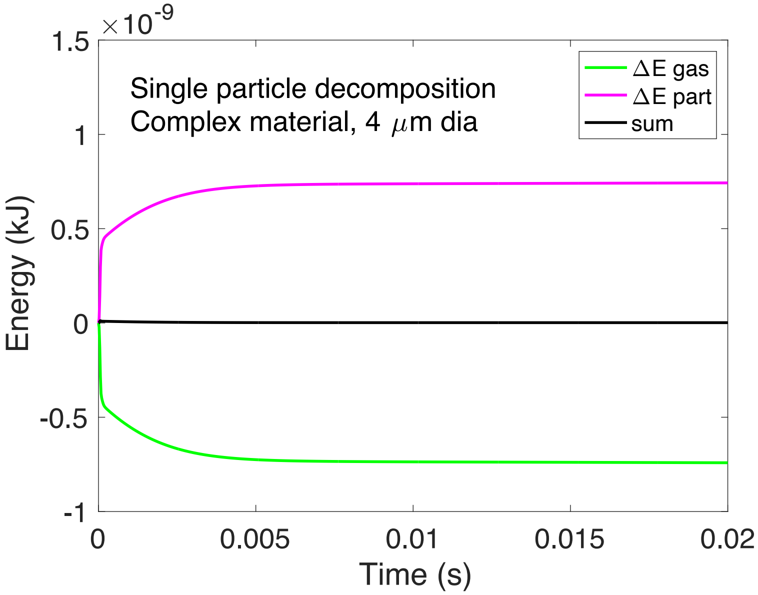






Energy budget verification test





1500 °C initial gas temperature
20 C
4 mm x 4 mm
4 μm particle
no radiation

Thermal Extinction Model

$$\mathit{Fuel} + \mathit{Air} \longrightarrow \mathit{Products}$$

$$\tilde{\phi} \equiv \min\left(1, \frac{sZ_F^0}{Z_A^0}\right) = \frac{Z_A^0 - Z_A}{Z_A^0}$$

$$(1-\tilde{\phi})(Z_A^0 + Z_P^0)$$

Excess Air and Products removed from stoichiometric pocket of reactants

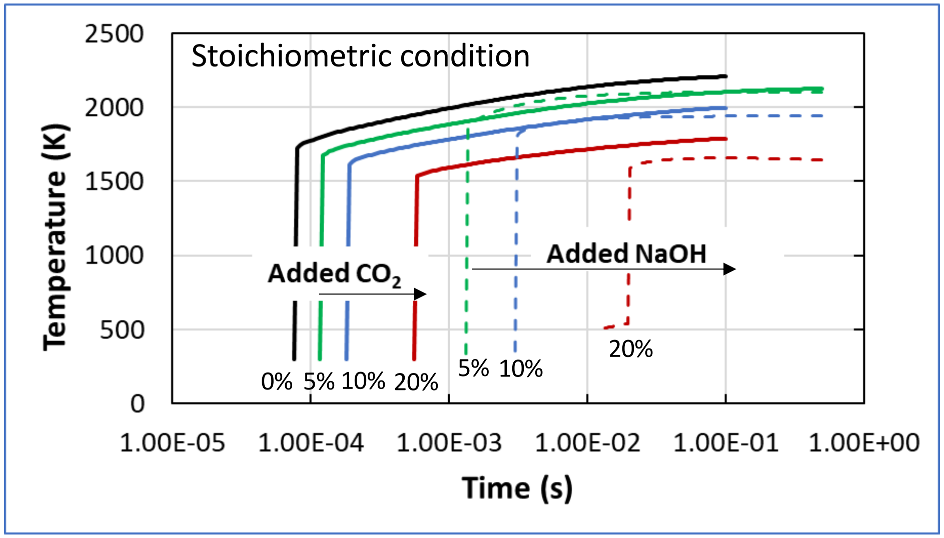
$$\boxed{Z_F^0\, h_F(T) + \tilde{\phi}\, Z_A^0\, h_A(T) + \tilde{\phi}\, Z_P^0\, h_P(T) \; < \; Z_F\, h_F(T_{CFT}) + \left[Z_P - (1-\tilde{\phi})\, Z_P^0\right] h_P(T_{CFT})}$$

Defines an extinction event

Propane-Air PSR Computations

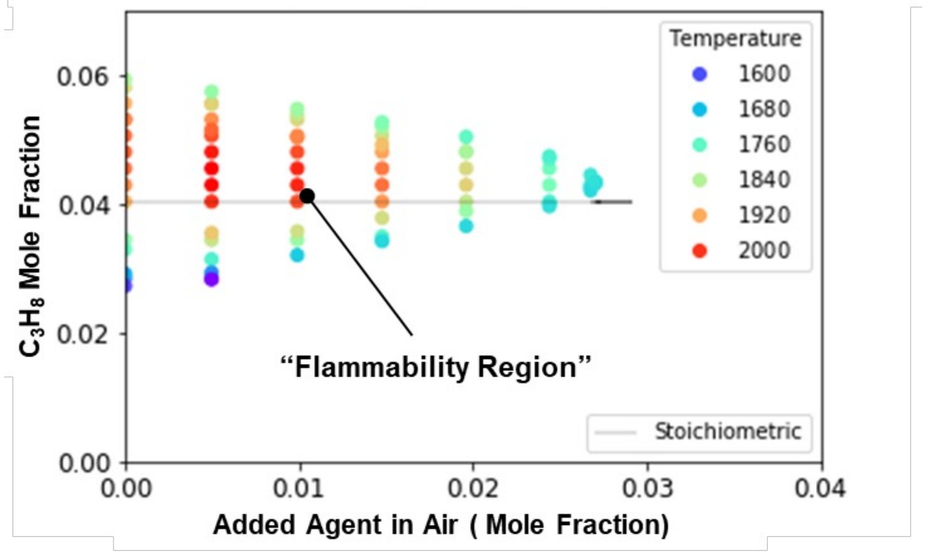
- Zero-dimensional, steady state, constant pressure reactor
- Detailed Propane/Na chemical kinetics
- Na species ($NaHCO_3$, Na, NaOH, $(NaOH)_2$, NaO, NaH, Na_2O_2, Na_2O, NaO_2)

Reactor temperature versus residence time



- Temperature decreases with decreased residence time
- Reaction does not occur below critical residence time (extinction)

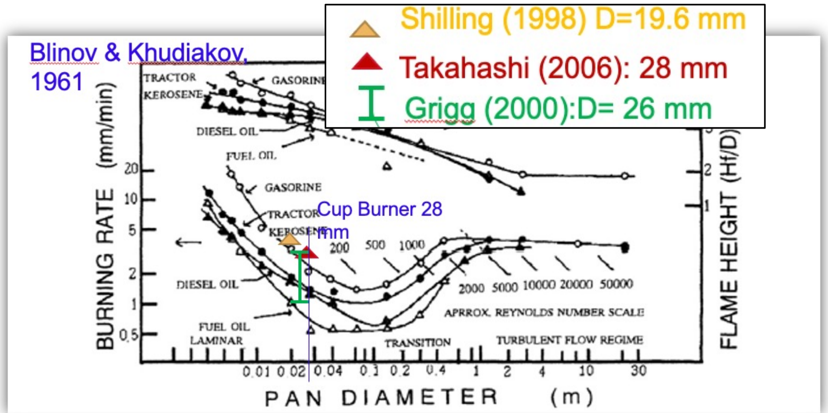
Residence time = 0.3 ms



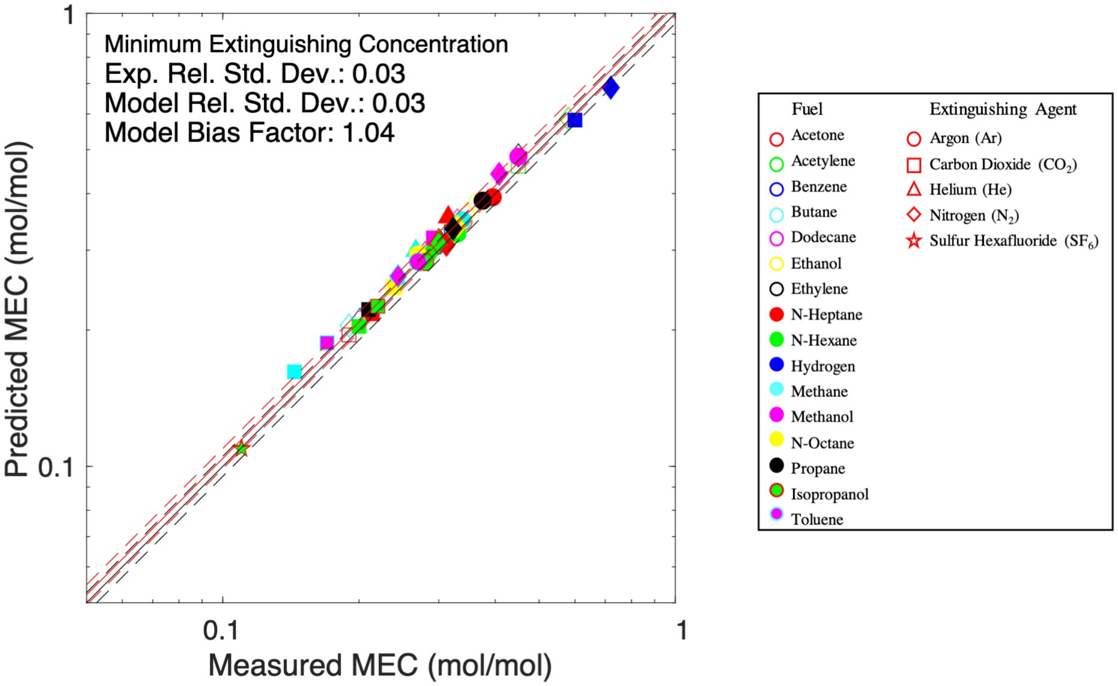
- Added agent = 1:1 NaOH/CO_2 mixture

Validation Cases

- Gaseous agents (FDS validation guide)
- Free burning heptane cup
- Heptane with Water Mist (Shilling)
- **Propane with $NaHCO_3$ (Hamins)**
- Heptane with $NaHCO_3$ (Hamins)

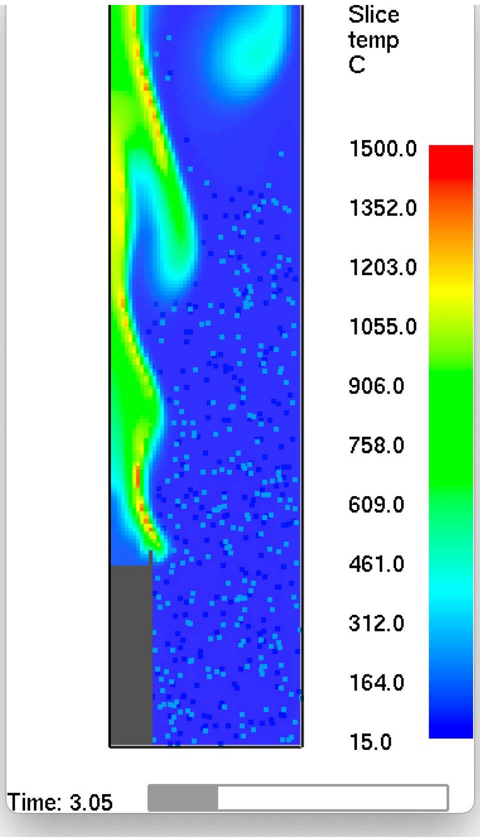


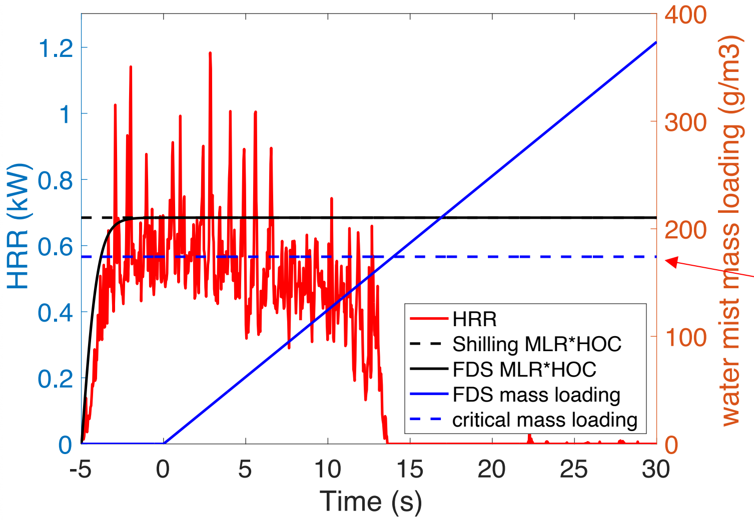
The simulated cup burner size (D= 0.028 m) is in laminar flame region

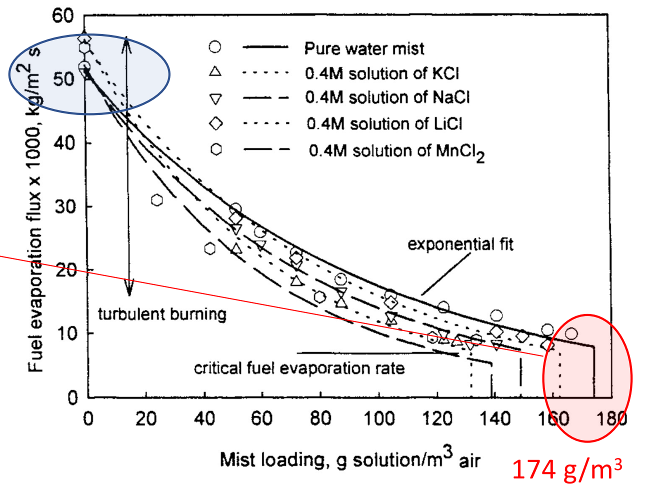


CFT taken from STANJAN calculations with stoich fuel and air diluted with MEC of gaseous agent.

Shilling et al. (1998) n-heptane with water mist







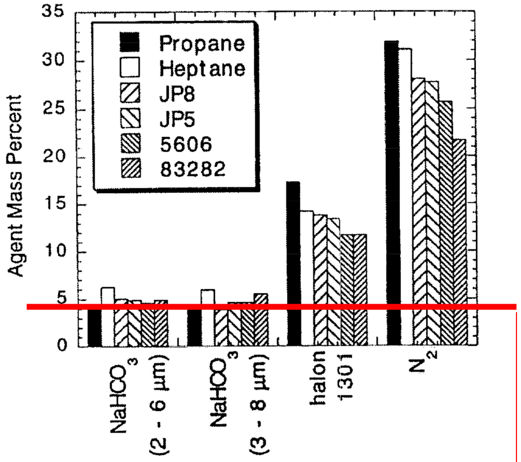
from Shilling et al. (1998)

174 g/m³ critical mass loading

Simulation details:

- “LES”, dx=1 mm
- specified fuel flow rate (0.05 kg/m2/s)
- AIT and CFT taken from literature
- small pilot zone just above cup (AIT=0 K)
- default radiation parameters
- specified radiative fraction, 0.40
- particle D_{50} = 8.2 μm (Shilling)
- Rosin-Rammler/lognormal distribution

Injection of MEC of CO2 and NaOH

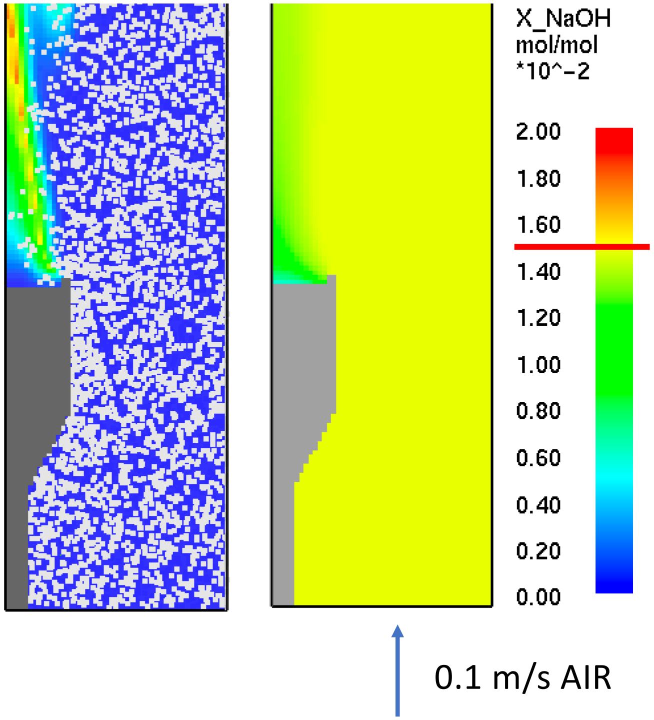


Minimum Extinguishing Concentration

$$\boxed{\mathrm{MEC} = 4.2\ \%}$$

by mass

$$X_{\mathrm{NaOH}} = 0.015$$



$$Y_{agent} = \frac{\dot{m}''_{agent}}{\dot{m}''_{air} + \dot{m}''_{agent}}$$

$$\dot{m}''_{agent} = \frac{\dot{m}''_{air}}{100/\mathrm{MEC} - 1}$$

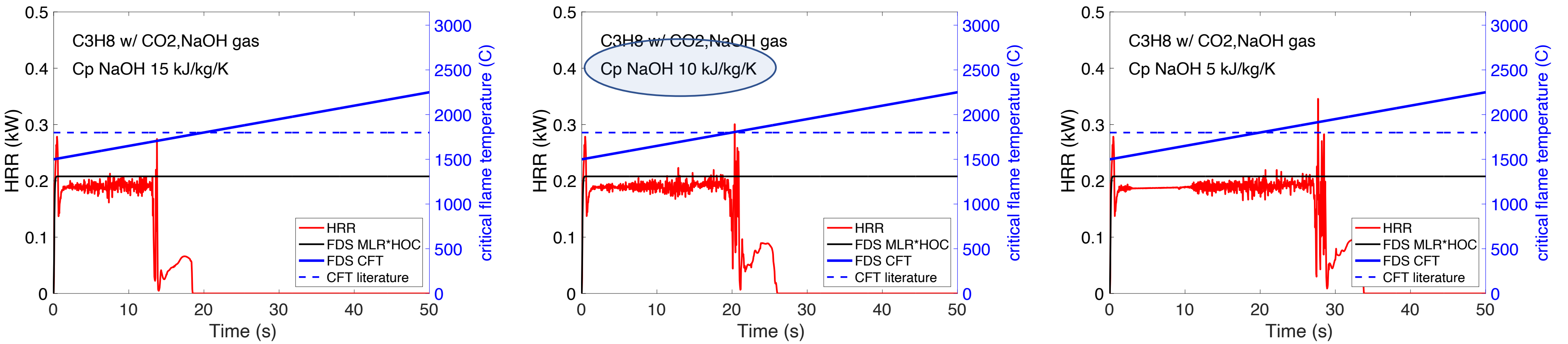
$$\dot{m}''_{agent} = \frac{(1.2\ \mathrm{kg/m^3})(.1\ \mathrm{m/s})}{100/4.2 - 1}$$

$$= 0.0053\ \mathrm{kg/m^2/s}$$

$$\dot{m}''_{\mathrm{CO_2}} = 0.0028\ \mathrm{kg/m^2/s}$$

$$\dot{m}''_{\mathrm{NaOH}} = 0.0025\ \mathrm{kg/m^2/s}$$

Adjustment of NaOH Specific Heat



NaOH **Cp=10 kJ/kg/K** achieves extinction at 1800 °C

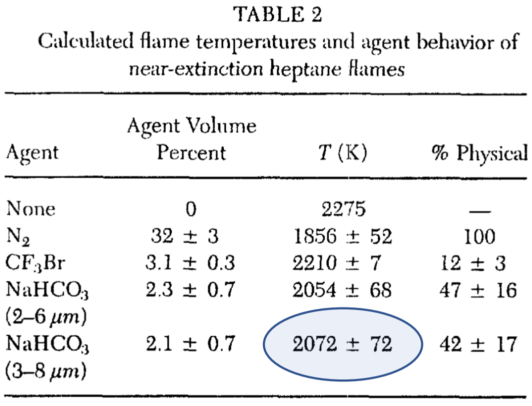


TABLE 2
Calculated flame temperatures and agent behavior of *near-extinction heptane flames*

Agent	Agent Volume Percent	*T* (K)	% Physical
None	0	2275	—
N_2	32 ± 3	1856 ± 52	100
CF_3Br	3.1 ± 0.3	2210 ± 7	12 ± 3
$NaHCO_3$ (2–6 *μm*)	2.3 ± 0.7	2054 ± 68	47 ± 16
$NaHCO_3$ (3–8 *μm*)	2.1 ± 0.7	2072 ± 72	42 ± 17

from A. Hamins (1998)

LES with flame heat transfer model

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&COMB SPEC_CHEM_ID='NaOH', SPEC_CHEM_CP_FAC=1000/
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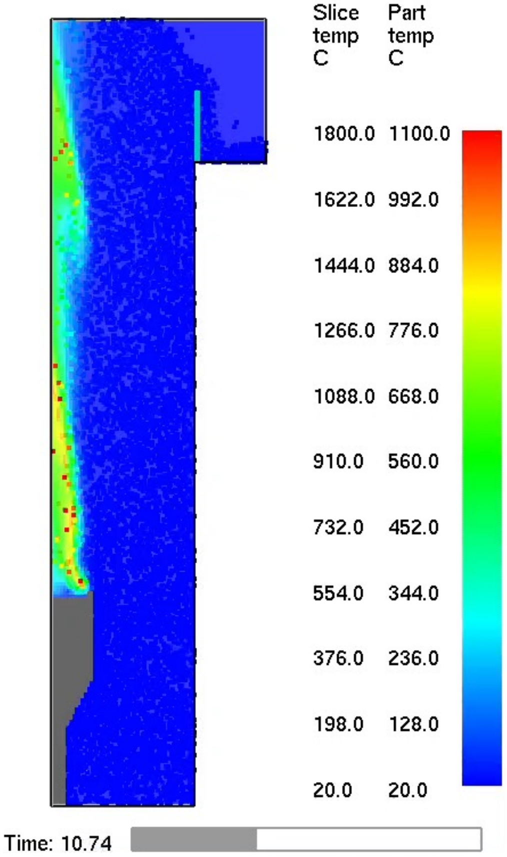
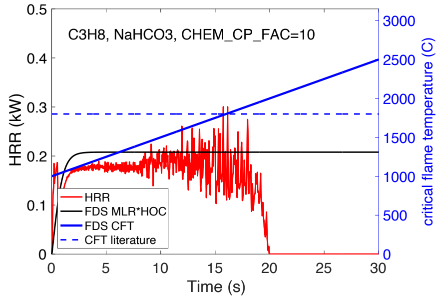
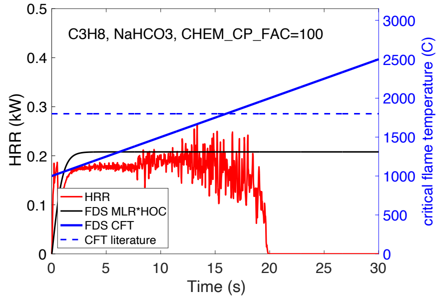
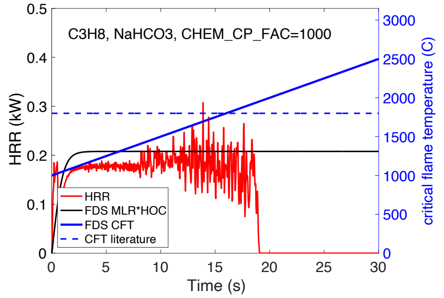




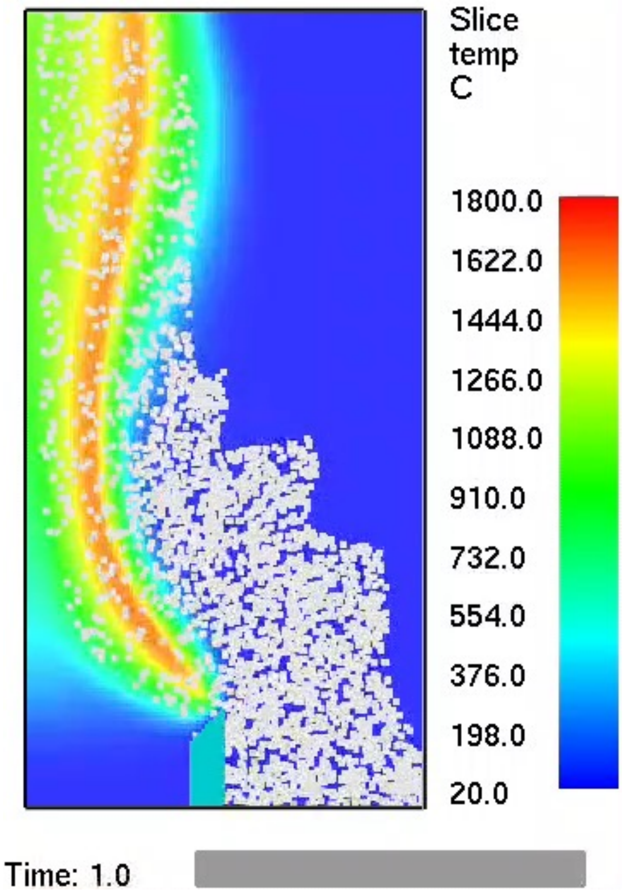


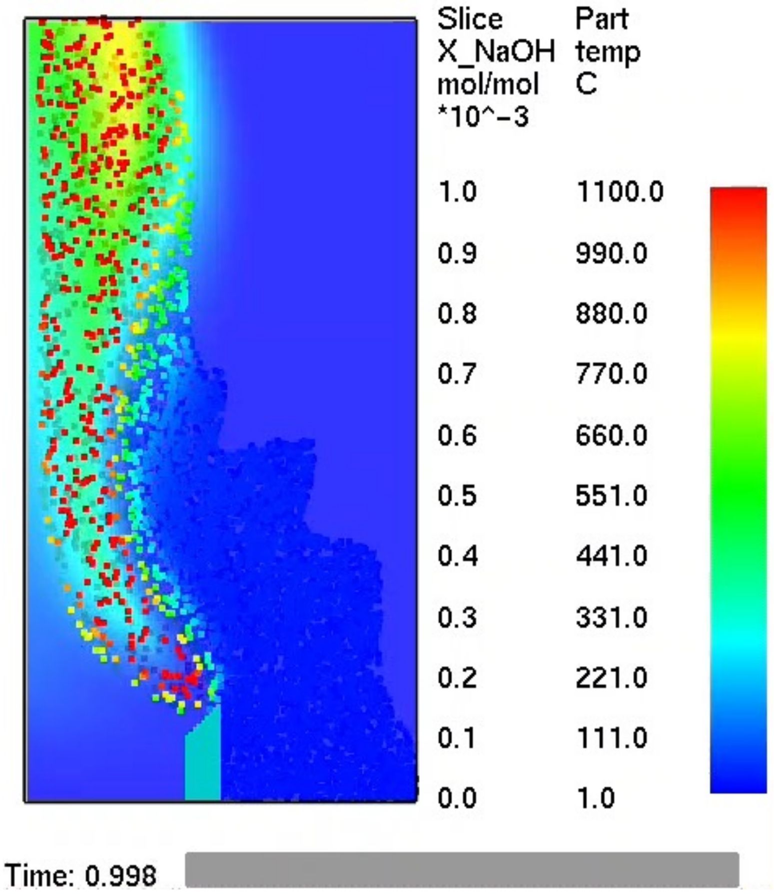


Basically, no effect.

Flame extinguishes with CFT near adiabatic flame temperature.

DNS (dx=0.2 mm)

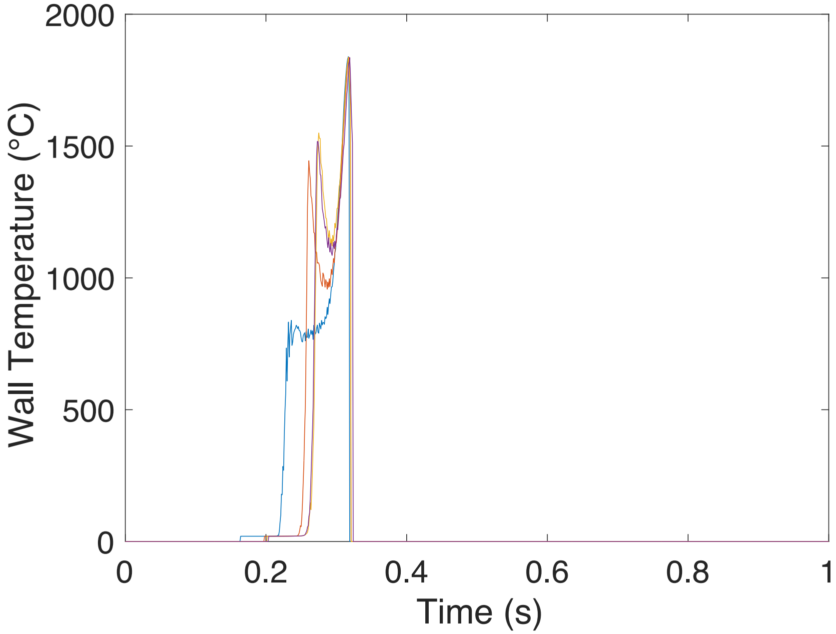

Slice
temp
C
1800.0
1622.0
1444.0
1266.0
1088.0
910.0
732.0
554.0
376.0
198.0
20.0
Time: 1.0


Slice
X_NaOH
mol/mol
*10^-3
Part
temp
C
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
1100.0
990.0
880.0
770.0
660.0
551.0
441.0
331.0
221.0
111.0
1.0
Time: 0.998

DNS temperature time history for particles

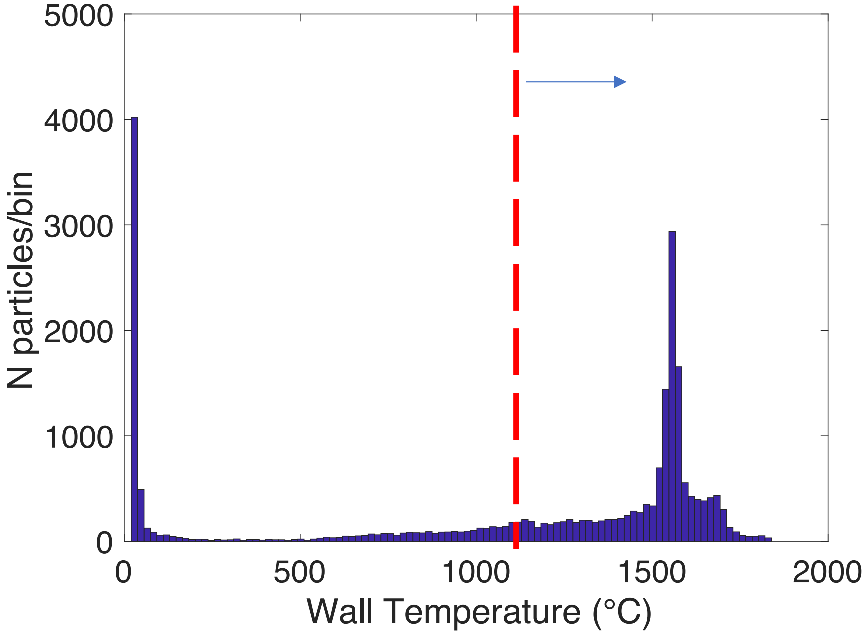
22,589 particles

Tmax > 1835 C
4/22589

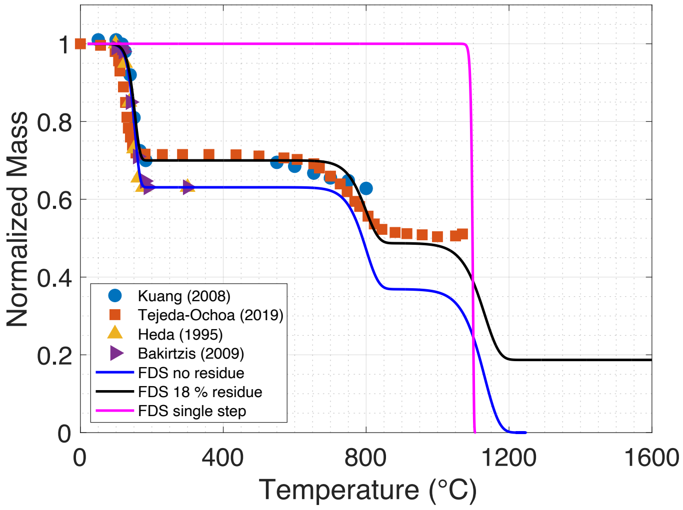


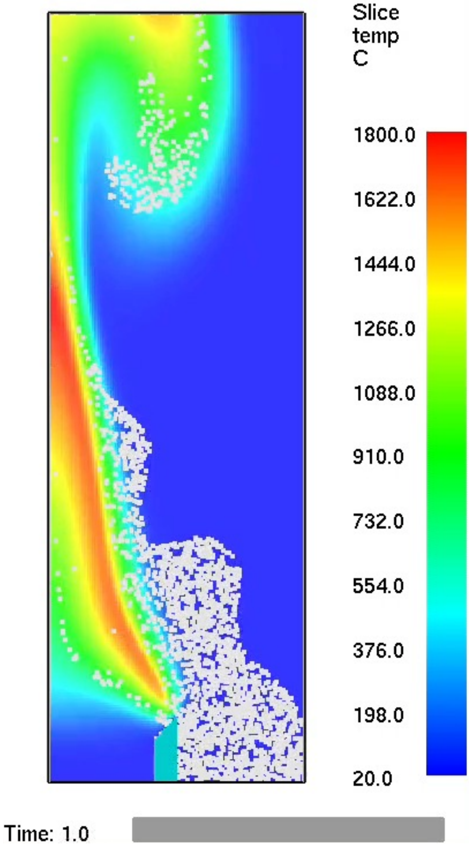
no time shift

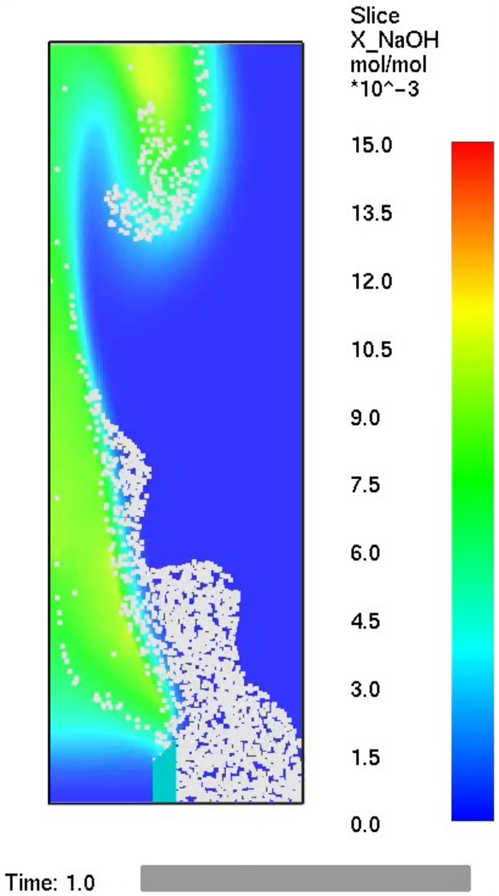
Tmax > 1100 C
14893/22589 (65 %)



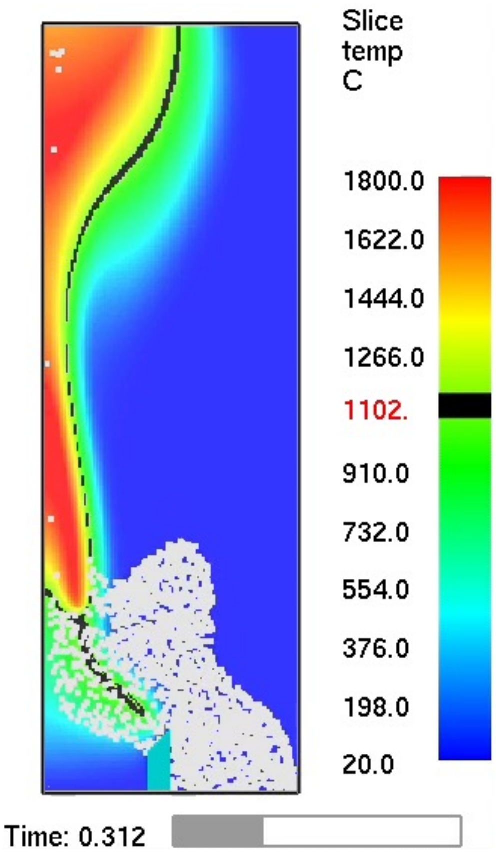
DNS 1 step fast at 1100 °C, CFT=1447 °C

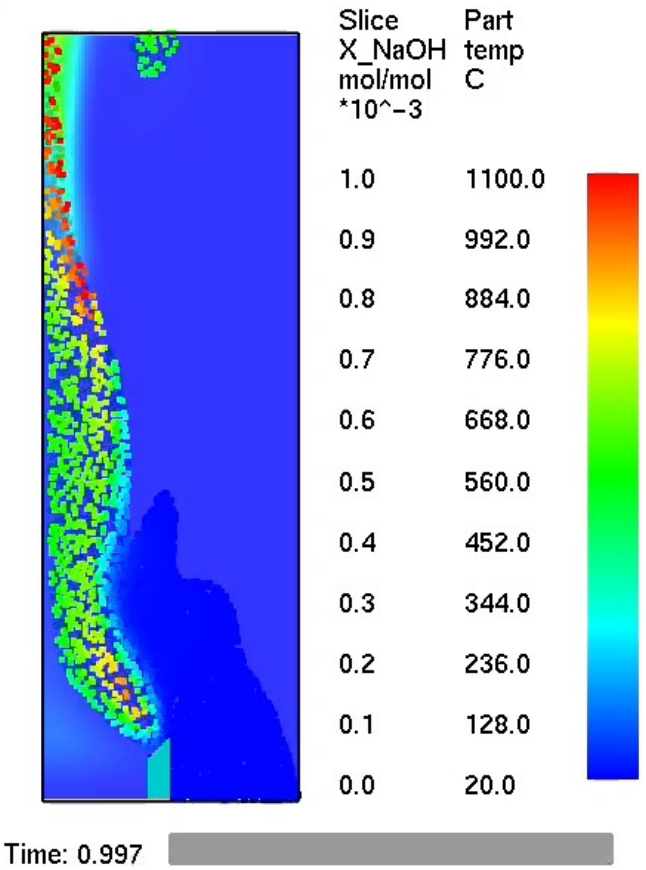


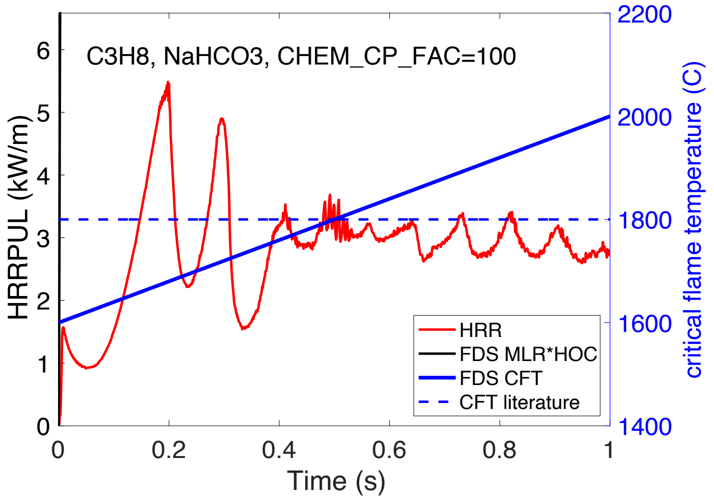




DNS 1 step fast, ramp CFT







Conclusions

- We have proposed a simple modification of the FDS thermal extinction model---adjustment of the agent specific heat---to mimic the effect of chemistry from gaseous NaOH in sodium bicarbonate suppression.
- We have shown proof of concept by assuming full particle decomposition and injecting the corresponding MEC of the NaOH agent as a gas.
- The kinetics of the final step do not appear to be a significant limitation. The larger problem lies in generating sufficient NaOH.
- The final particle decomposition step occurs at around 1100 °C. The particle decomposition is endothermic and cools the flame, making numerical modeling of the final particle decomposition step challenging.
- Attempts to cool the flame below the NaOH decomposition temperature (1100 °C) have been unsuccessful.