

BESS Deflagration Modeling and Hazard Prevention

Ofodike A. Ezekoye
Dept. of Mechanical Engineering
University of Texas at Austin

**Energy Storage Systems Safety &
Reliability Forum 2022**

UT Fire Research Group:
Erik Archibald, Sam Matthews, Robert
Kennedy, Serhat Bilyaz, Kevin Marr, Austin
Baird

Overview of Talk

- Deflagration Awareness
- Modeling Considerations
- Hazard Prevention
- Summary

BESS Explosions

4 out of 42 ESS incidents on BESS Failure Event Database¹ were explosions.

The other 38 were fires.

Surprise, AZ USA



Beijing, China



Liverpool, UK



Griffith University



¹EPRI BESS Failure Event Database:

https://storagewiki.epri.com/index.php/BESS_Failure_Event_Database

Residential Deflagration Safety



<https://sanfrancisco.cbslocal.com/2019/06/08/fairfield-garage-fire-sends-5-first-responders-hospital/>



DOE Empowered (NFPA, Argonne, Amphenol, UL,...)



Geometries of Interest?

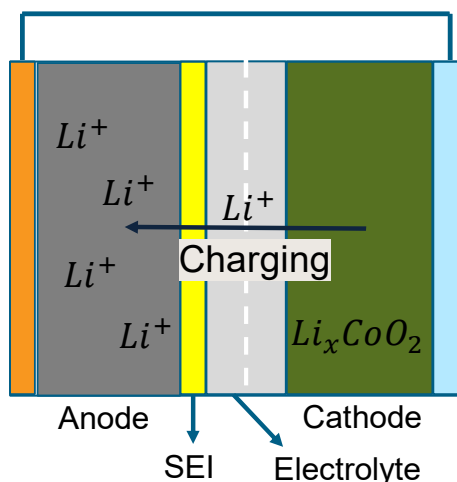


What about the chemistry allows flammable gas generation

Various exothermic reactions may take place in a battery both in anode or cathode side

Anode

1. SEI Decomposition
 - SEI protection is broken
 - Triggers the other reactions
2. SEI Regeneration
 - Consumes Li^+
 - Forms new SEI
3. Li^+ +Electrolyte Reaction
 - Generates hydrocarbons
4. Binder Decomposition

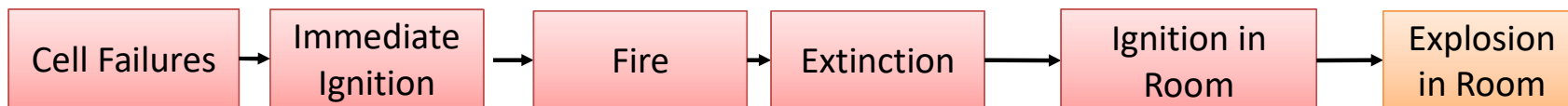


Cathode

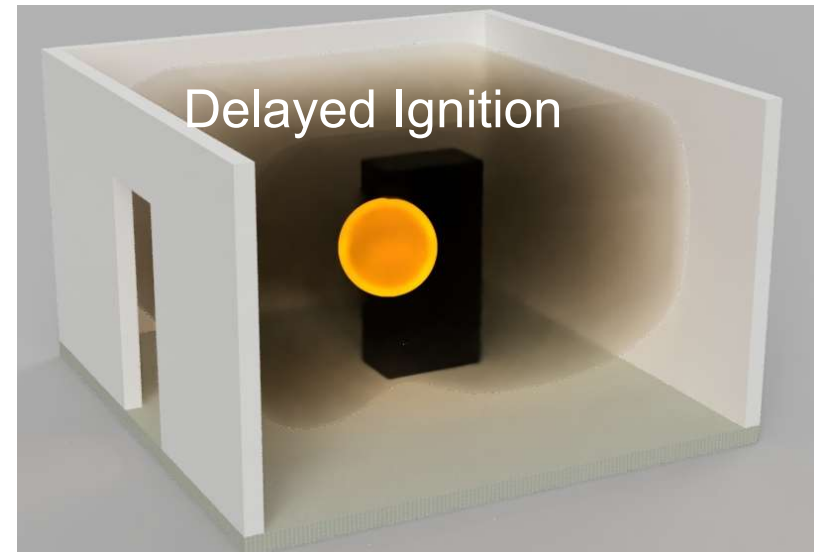
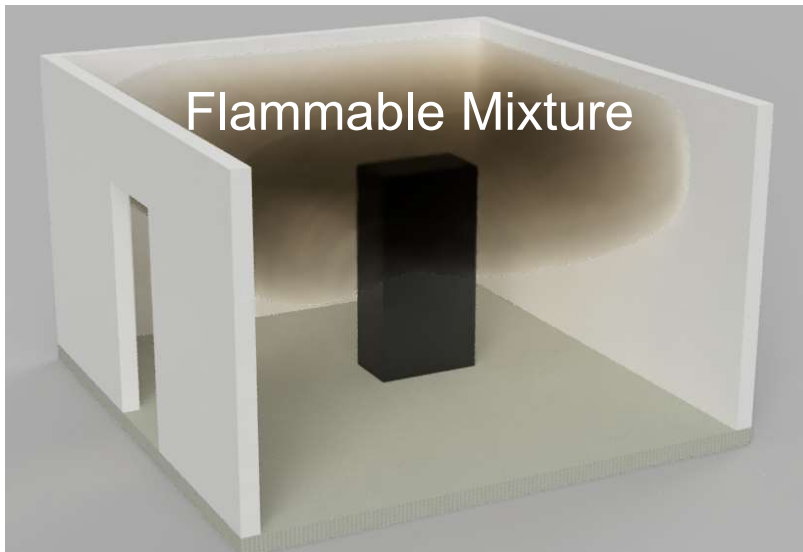
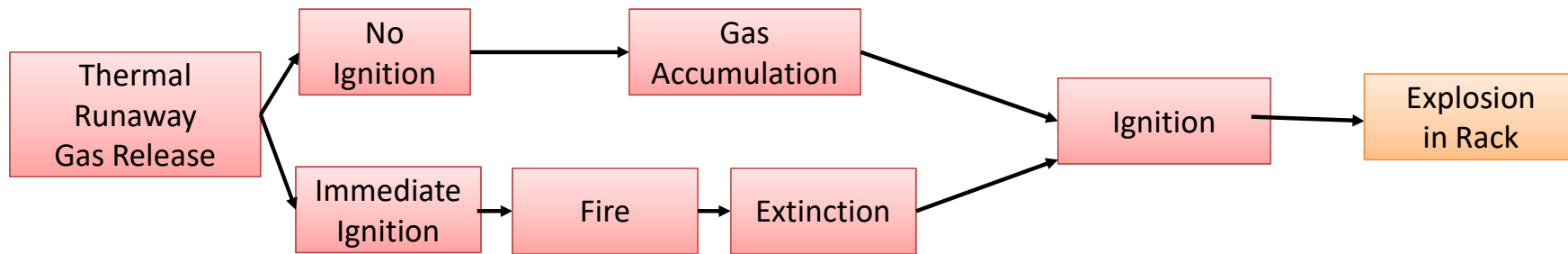
1. Cathode decomposes, releases oxygen and oxidizes electrolyte in multiple stages
2. Binder Decomposition

FAA FRC EXPERIMENT

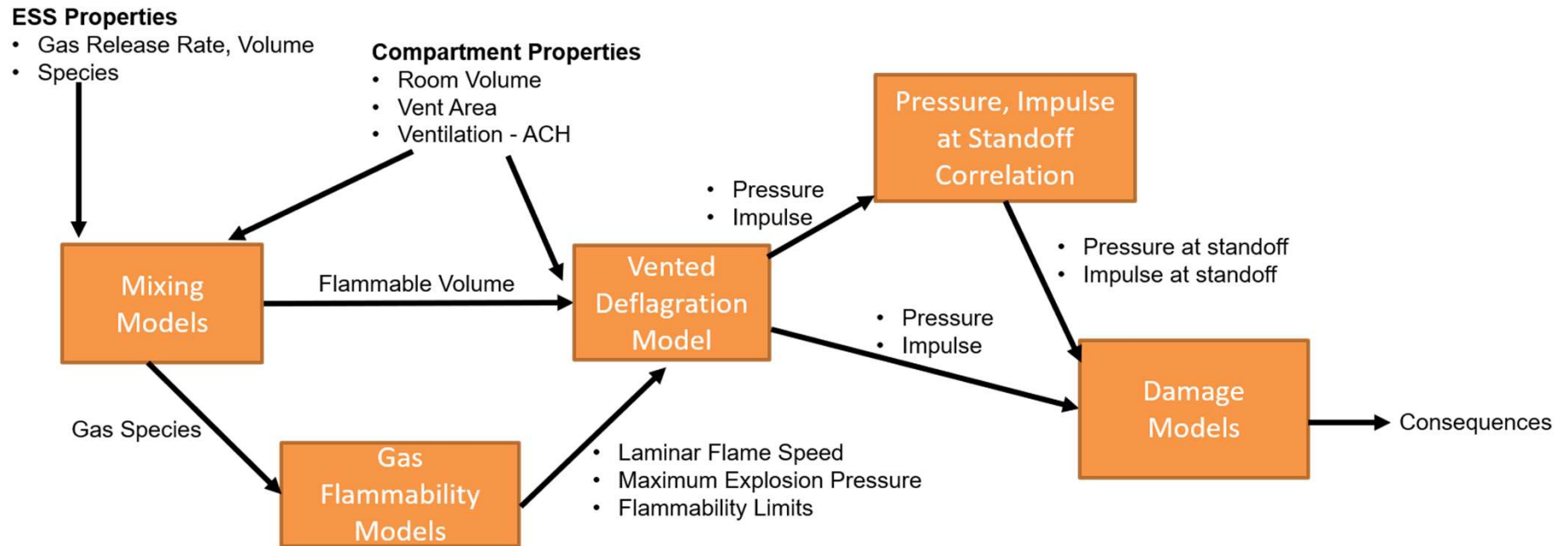
- 5000 18650 Cylindrical Cells
- ~ 40 kWh of energy storage
- Fire Resistant Container designed to limit oxygen to contain Class A fires
- Aerosol fire suppressant extinguished fire at about 20 minutes
- Explosion occurs after 45 minutes



Understanding the Hazard



Inputs and Models for Hazard Analysis



Parameters for Vented Gas Explosion

Release Attributes

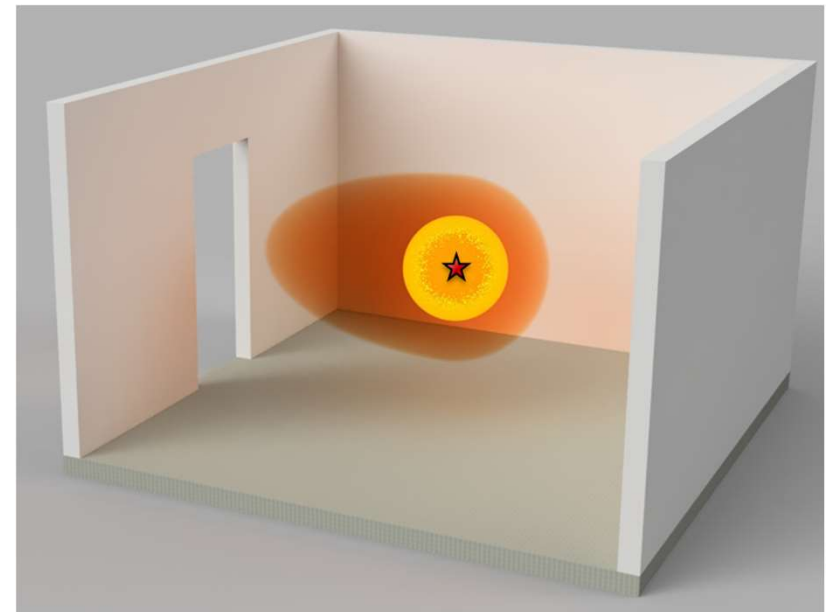
- Volume Released
- Mixing with gas

Gas Properties

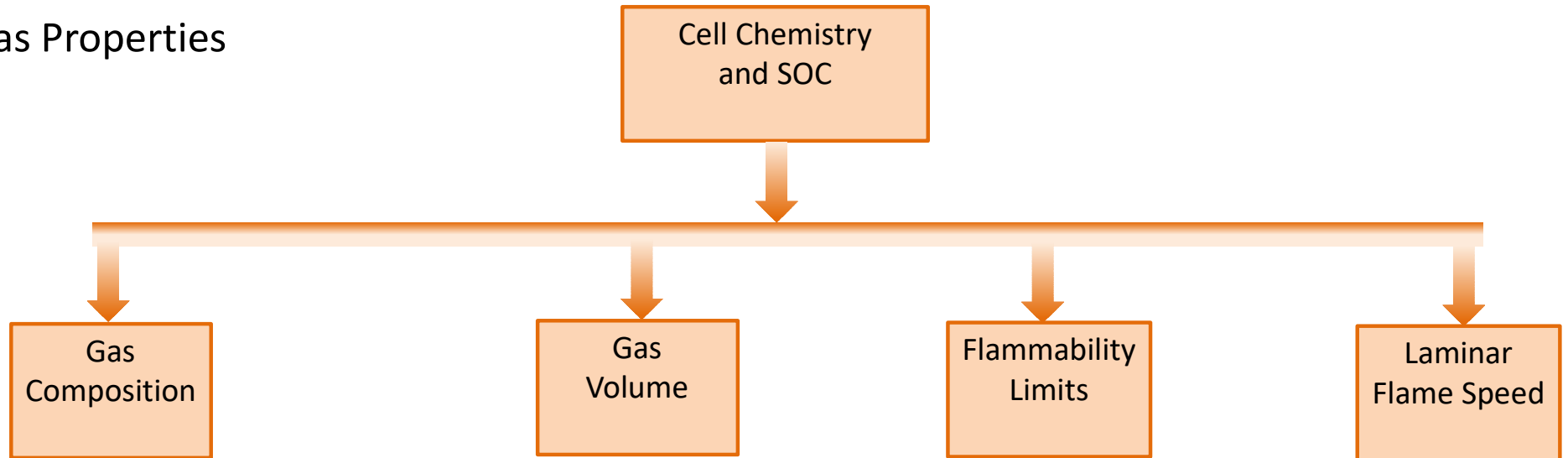
- LFL/UFL
- Flame Speed
- Maximum Pressure

Room Properties

- Volume
- Vent Area
- Geometry
- Obstructions



Gas Properties



Cathode	NMC	LCO
H ₂	33.9%	24.7%
CO	18.2%	14.7%
CH ₄	5.6%	5.0%
CO ₂	31.4%	44.0%
Total	89.1%	88.4%

LCO pouch cells

$$V \left[\frac{L}{Wh} \right] = 0.37 SOC^{1.9}$$

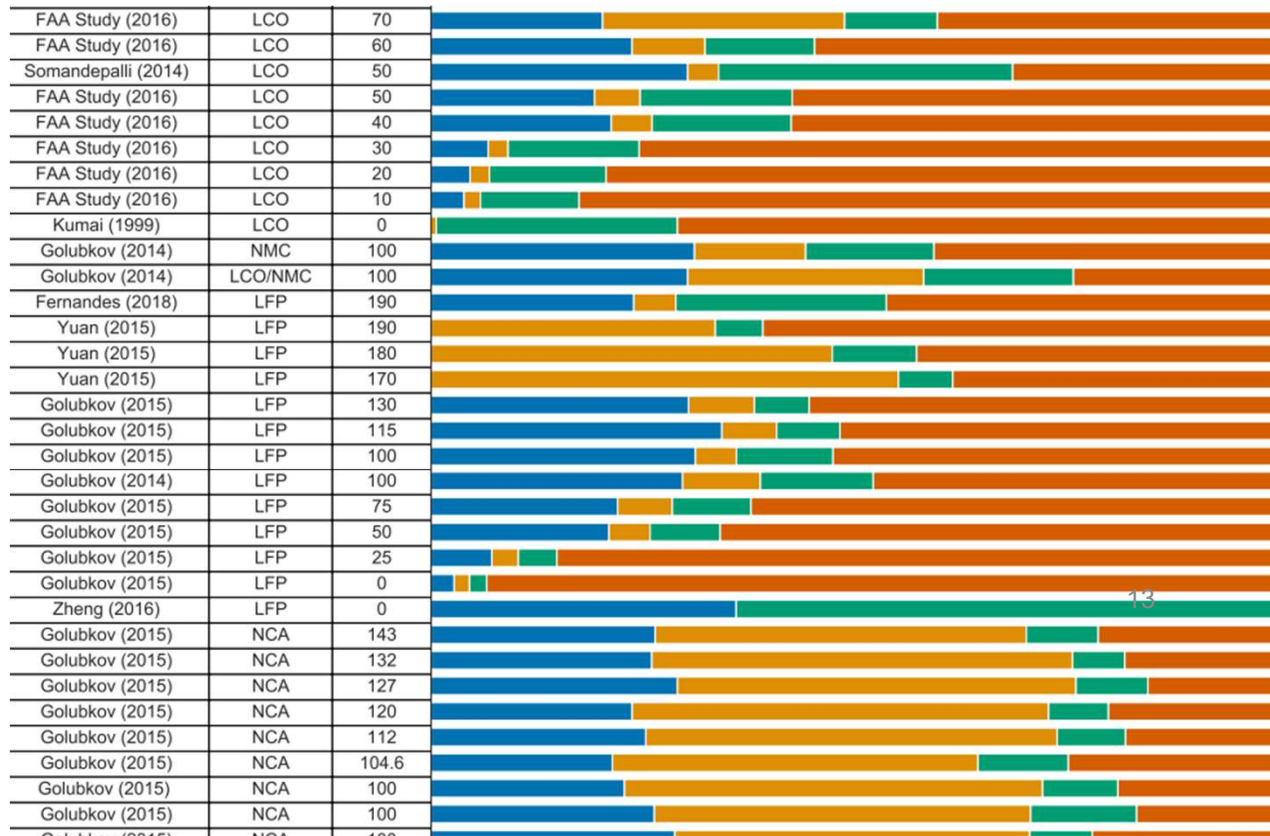
NMC pouch cells

$$V \left[\frac{L}{Wh} \right] = 0.47$$

Cell Chemistry	Lower Flammability Limit (%)
LCO	5.8 to 8.8
LFP	8.6 to 10.0
NCA	6.7 to 11.8

Deflagration Hazard:	Flame Speed (m/s)
Class 1 Dust: Sugar	–
Class 3 Dust: Aluminum	–
Propane	0.40
Hydrogen	2.80
LCO 100% SOC	0.49 - 0.65
LFP 100% SOC	0.37 - 0.42
NCA 100% SOC	0.69 - 1.07

Vent Gas Composition Literature Survey



Vent Gas Characterization

- Cantera: open-source chemical kinetics software
 - Lower Flammability Limit
 - Laminar Flame Speed
 - Maximum Over-Pressure
- Compared and Validated models with Literature



Cantera

Simple Model for Vented Gas Explosion

Mass Conservation

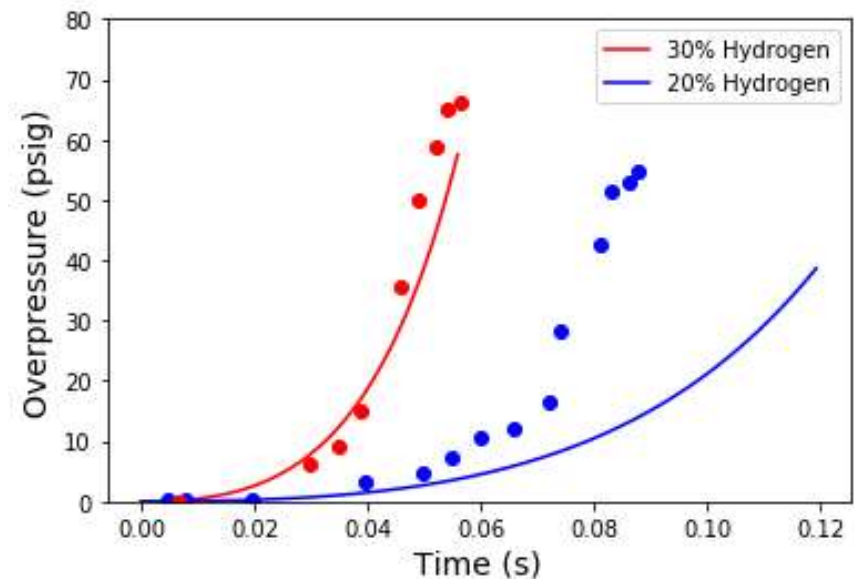
$$\frac{d}{dt} \left(\frac{m_u}{m_i} \right) + \frac{d}{dt} (n) + \frac{d}{dt} \left(\frac{m_v}{m_i} \right) = 0,$$

Energy Conservation

$$\frac{d}{dt} \left(\frac{m_u}{m_i} E_u \right) + \frac{d}{dt} (n E_b) + E_u \frac{d}{dt} \left(\frac{m_v}{m_i} \right) = 0.$$

Burning Rate

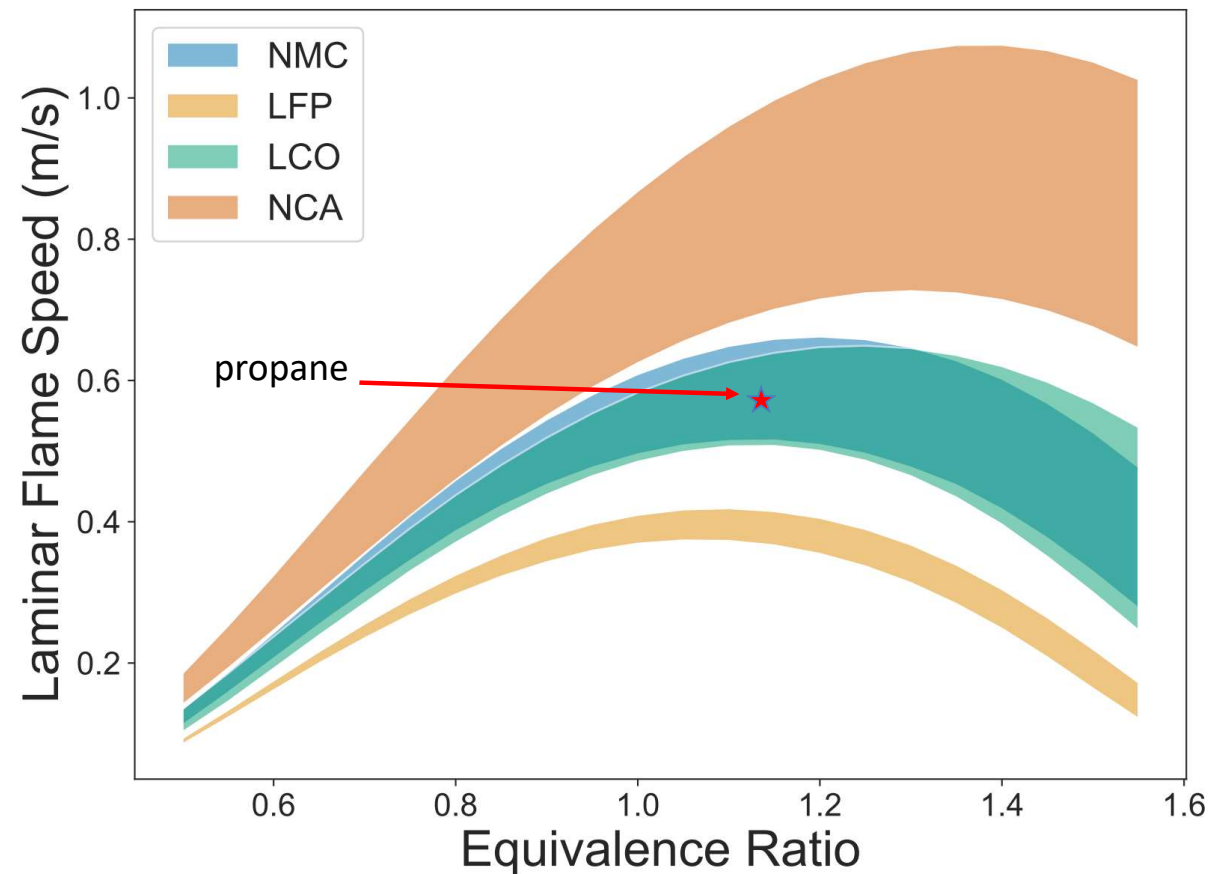
$$\frac{dn}{dt} = \frac{A}{V_i} \bar{S}_T \bar{p}^{1/\gamma_u} - K \frac{d}{dt} \left(\frac{m_v}{m_i} \right)_b$$



Pressure time history comparison between model and experiments for 2.3 m diameter sphere filled with hydrogen and air with central ignition.

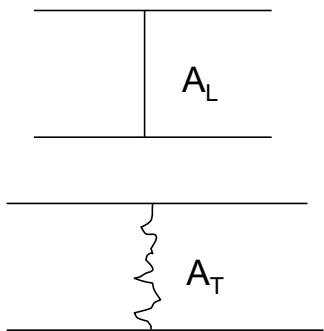
Estimated Flame Speeds

- Typical flame speed behavior for syngas type mixtures.
- A reasonable approximation is to use propane for NMC and LCO chemistries.



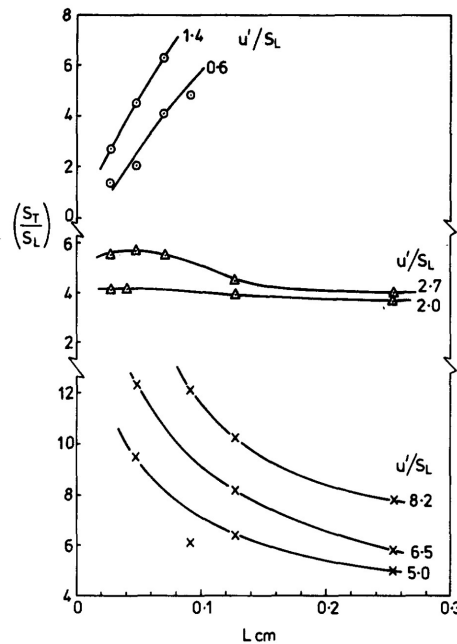
Turbulent Burning Rate

Unlike the laminar flame speed which is a fundamental physiochemical parameter for a given fuel-air mixture, the turbulent burning rate depends on system parameters to specify its value.

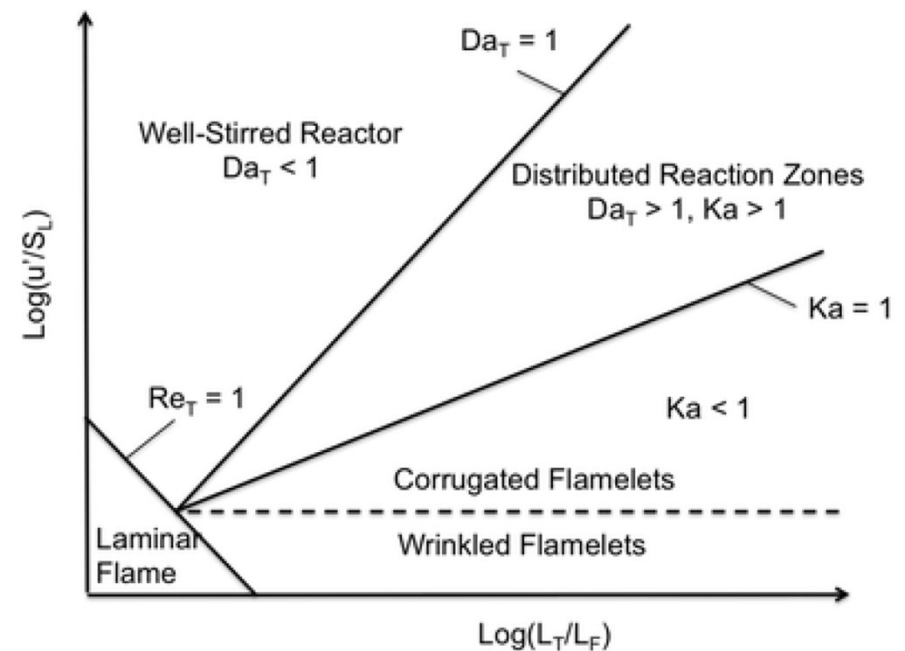


$$S_T/S_L = f(u'_0/S_L)$$

$$S_T/S_L = 1 + u'_0/S_L$$



Ballal, Dilip R., and Arthur H. Lefebvre. "Turbulence effects on enclosed flames." *Acta Astronautica* 1.3-4 (1974): 471-483.



NFPA 68

Lower Order Mitigation Models

Composition,
flame speed,
flammability limits

$$A_{v0} = \frac{A_s C}{\sqrt{P_{red}}}$$

Turbulence

$$C = \frac{S_u \rho_u \lambda}{2G_u C_d} \left[\left(\frac{P_{max} + 1}{P_0 + 1} \right)^{1/\gamma_b} - 1 \right] (P_0 + 1)^{1/2}$$

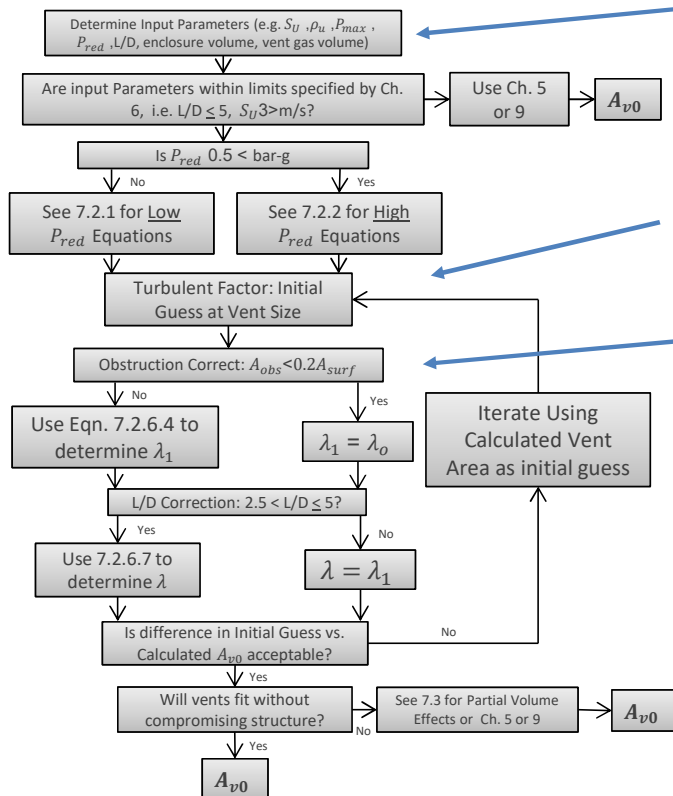
Obstructions

$$\lambda_0 = \varphi_1(\text{Re}_f) \varphi_2(\text{Re}_v)$$

$$\lambda_1 = \lambda_0 + [\lambda_0 f(A_{obs}/A_s) - \lambda_0] H_s(A_{obs}/A_s - 0.2)$$

$$\lambda = \lambda_1 + [\lambda_1 g(L/D) - \lambda_1] H_s(L/D - 2.5)$$

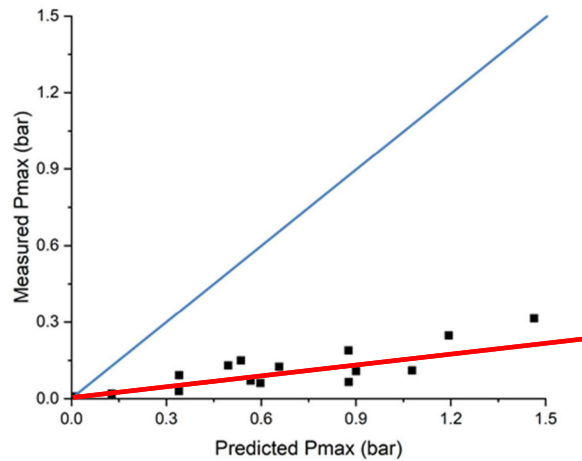
Obstruction and aspect ratio effects are identified.



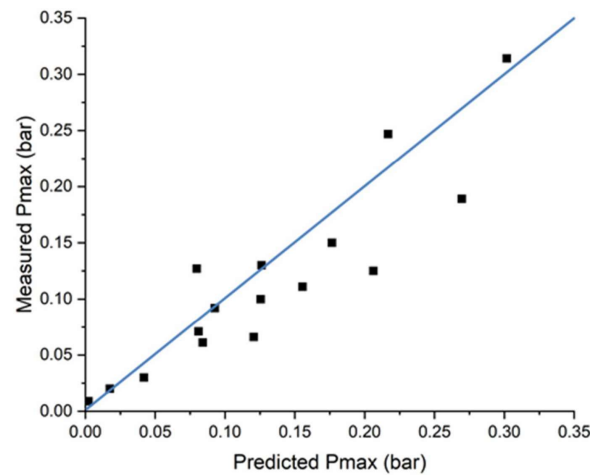
Epstein, Swift, & Fauske CNF 1986

“A major concern with the current standards (EN14994 [11] and NFPA 68 [12]) is that they are very conservative, which makes them not suitable to be used for low-strength enclosures.”

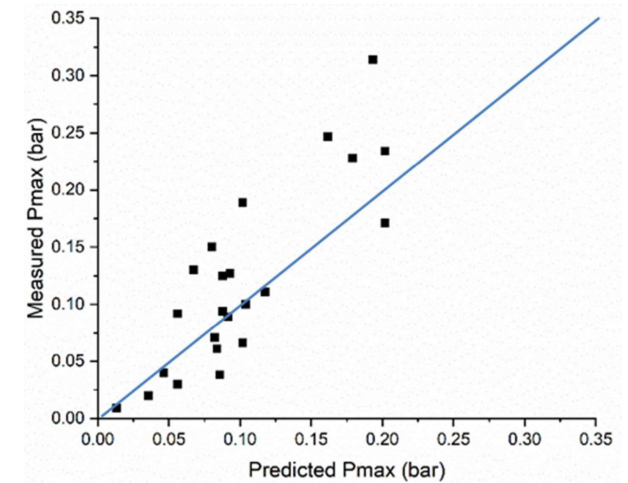
Modelling of Vented Explosion of Hydrogen-Air Mixtures by Sinha A., Wen J.*



(c) NFPA 68 [12].



(d) Bauwens model [4].



(e) Molkov model [10].

Model data input uses hydrogen cases with 76 experimental data points

Molkov & Bragin, Hydrogen air deflagrations: Vent sizing correlation for low-strength equipment and buildings, International Journal of Hydrogen Energy, 40 (2015)

NFPA 68 is not always conservative.

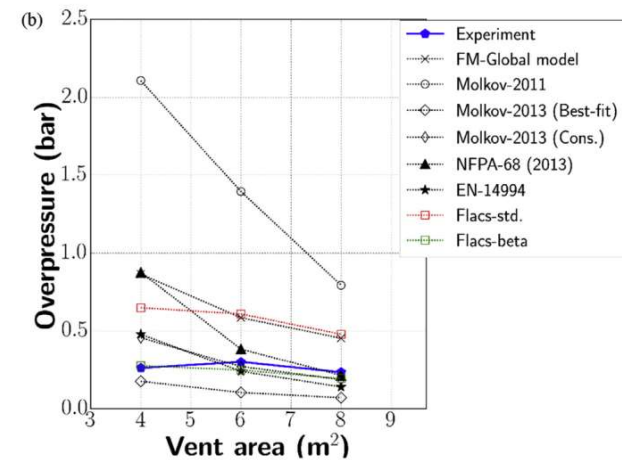
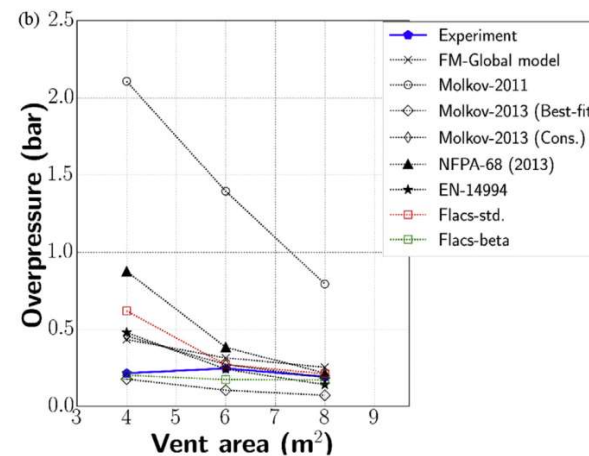
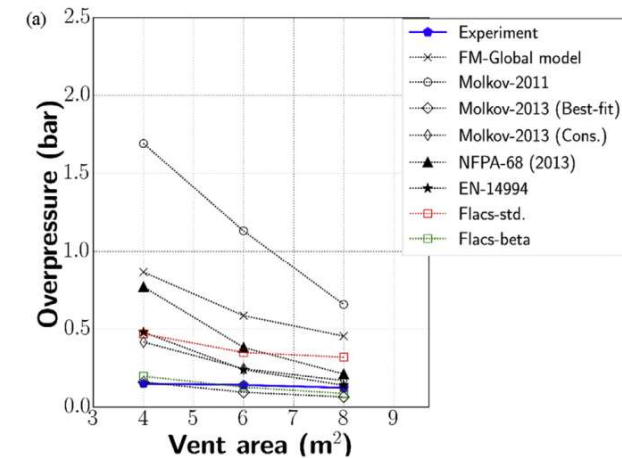
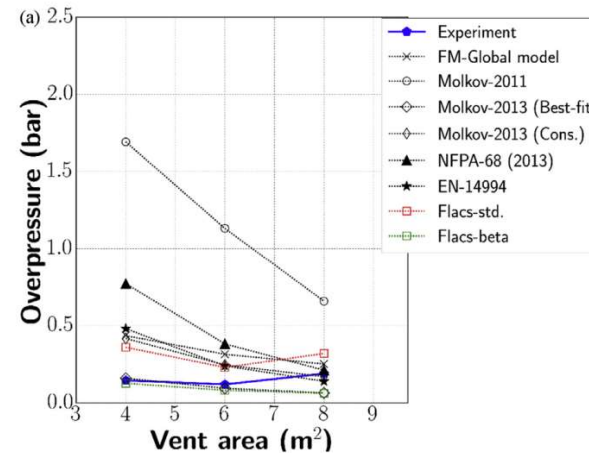
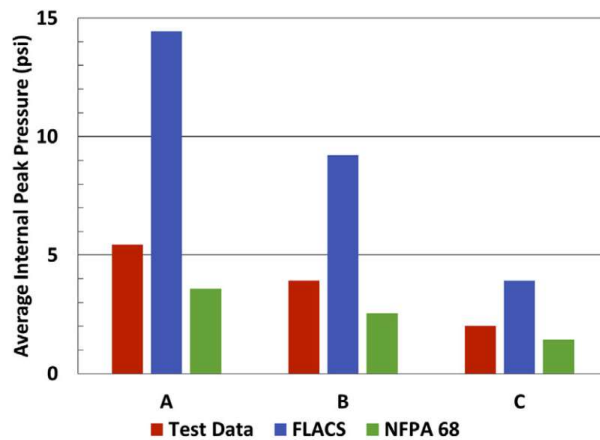


Fig. 15. Average internal peak pressure compared to FLACS simulations and NFPA 68 (2018).

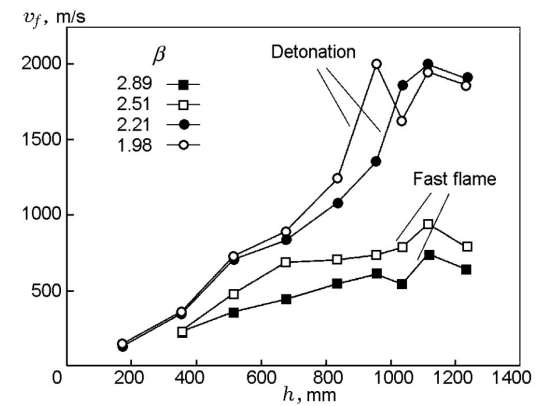
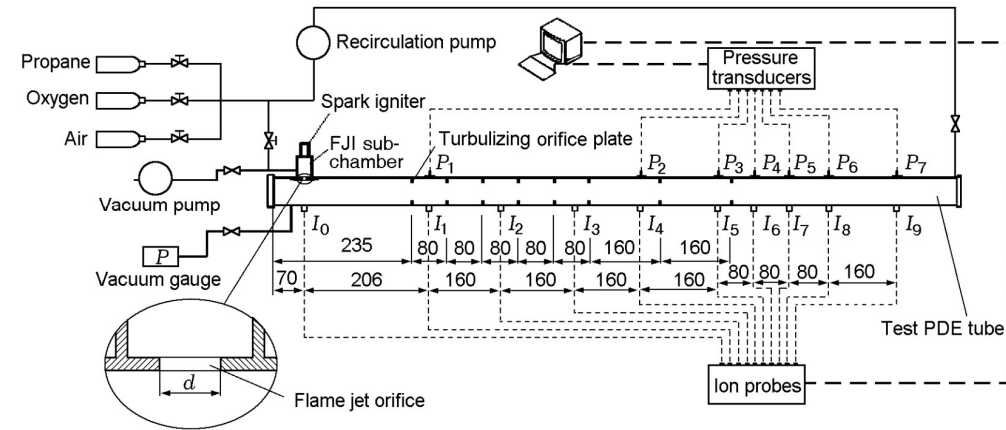
Diakow, Thomas, Vivanco, "Comparison of large-scale vented deflagration tests to CFD simulations for partially congested enclosures", Journal of Loss Prevention in the Process Industries Volume 56, November 2018

Lakshmipathy, Skjold, Hisker, Atanga, Consequence models for vented hydrogen deflagrations: CFD vs. engineering models

Limitations

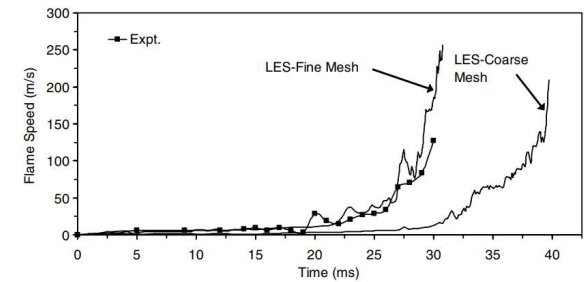
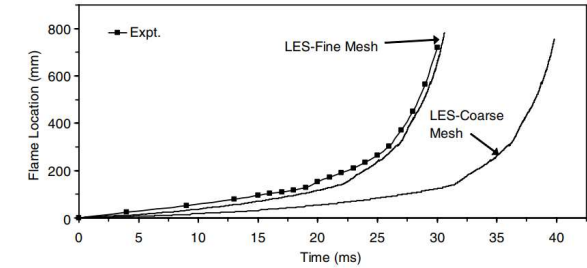
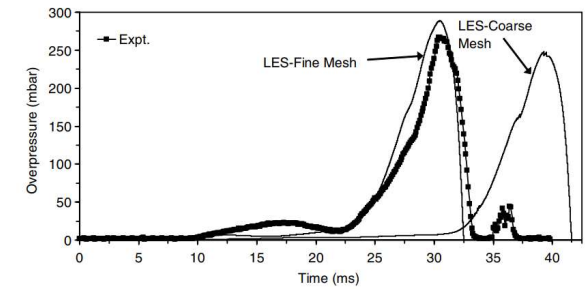
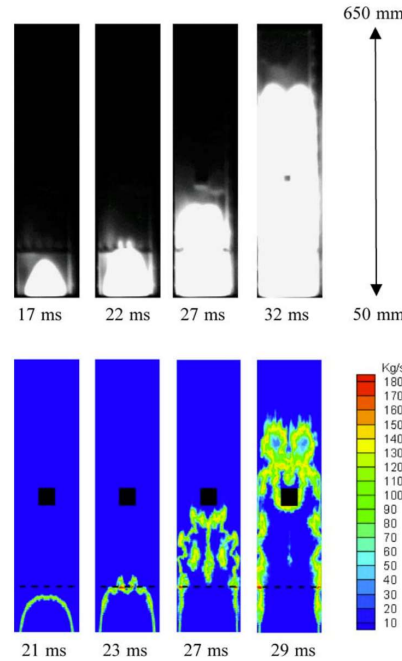
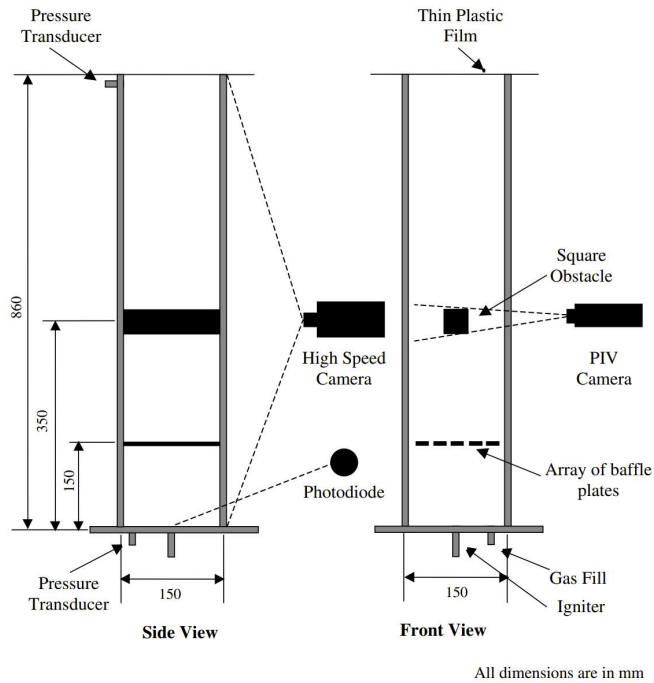
7.2.6.8 Equations for determining λ shall be subject to the following limitations:

The enclosure is isolated from possible flame jet ignition and pressures caused by a deflagration in an interconnected enclosure.



Zhao et al. used a turbulent propane jet flame to initiate fast turbulent flames and detonations in a channel





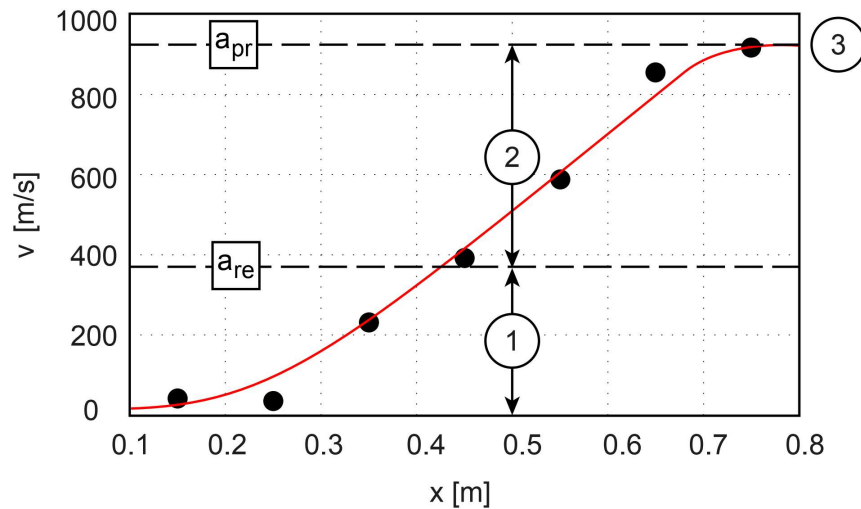
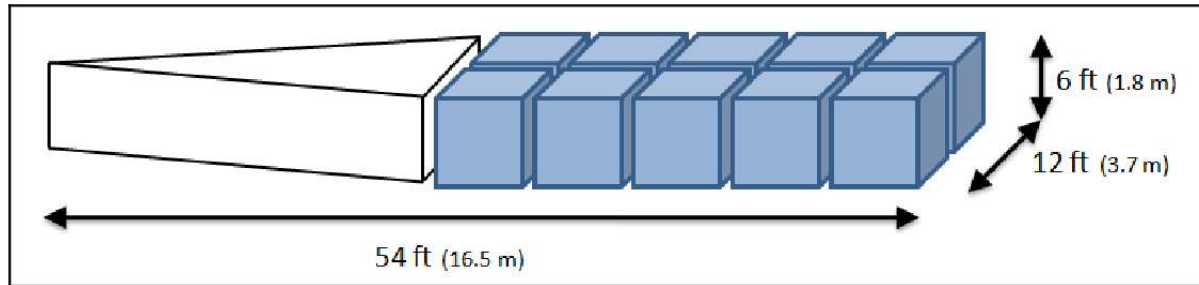
Test cases investigated experimentally with unsteady premixed flames

Case	Obstruction type and size	Area blockage ratio (%)	Array of baffle plates	Peak overpressure (mbars)	Time of peak overpressure (ms)	Terminal flame speed (m/s)
NONG	Nil	0	Nil	30	35.0	46
S1NG	Square, 37.5 mm	25	Nil	138	39.0	100
S1G1 ^a	Square, 37.5 mm	25	5 × 11 mm strips	265	30.5	130
S2NG	Square, 60 mm	40	Nil	185	36.0	93
S2G1	Square, 60 mm	40	5 × 11 mm strips	360	30.6	140
C1NG	Cylinder, 75 mm	50	Nil	188	37.5	95
C1G1	Cylinder, 75 mm	50	5 × 11 mm strips	280	30.4	130

^a Case for which LES calculations are performed.

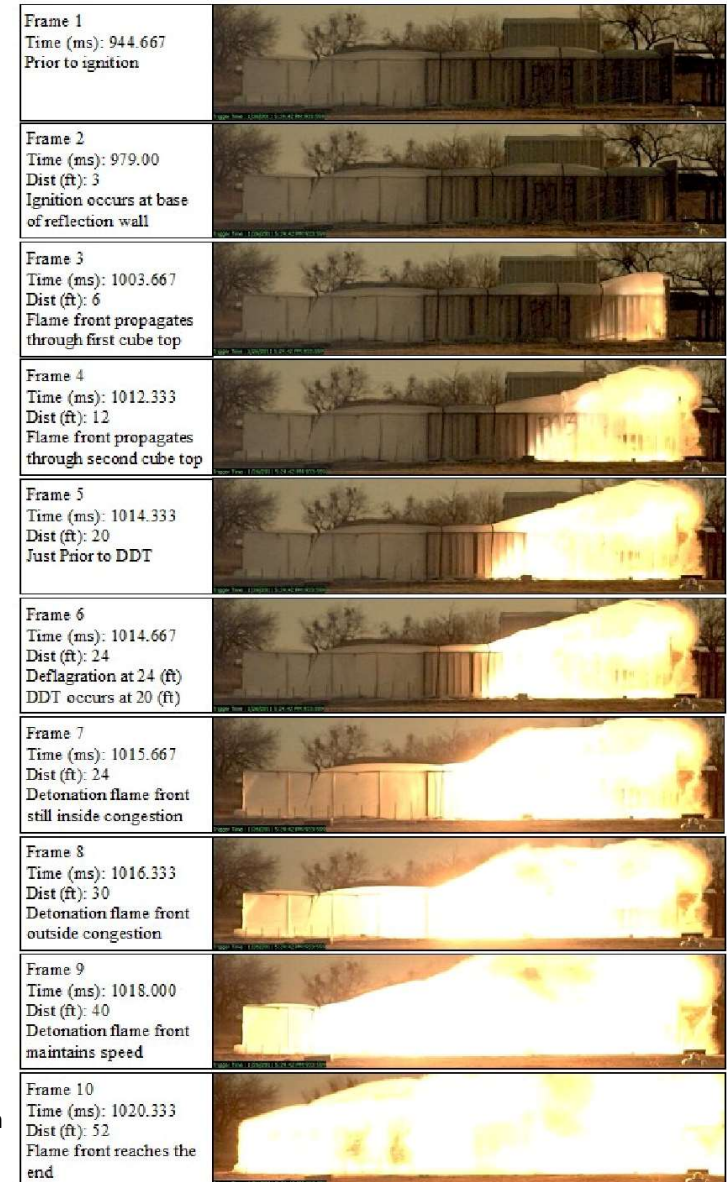
Measurements and large eddy simulation of propagating premixed flames
Masri, Ibrahim, Cadwallader

Still Frames from High Speed Video Illustrating Flame Front Propagation & Acceleration



Lorenz Rupprecht Böck, Deflagration-to-Detonation Transition and Detonation Propagation in H₂-Air Mixtures with Transverse Concentration Gradients, PhD Diss. TU-Munich 2015

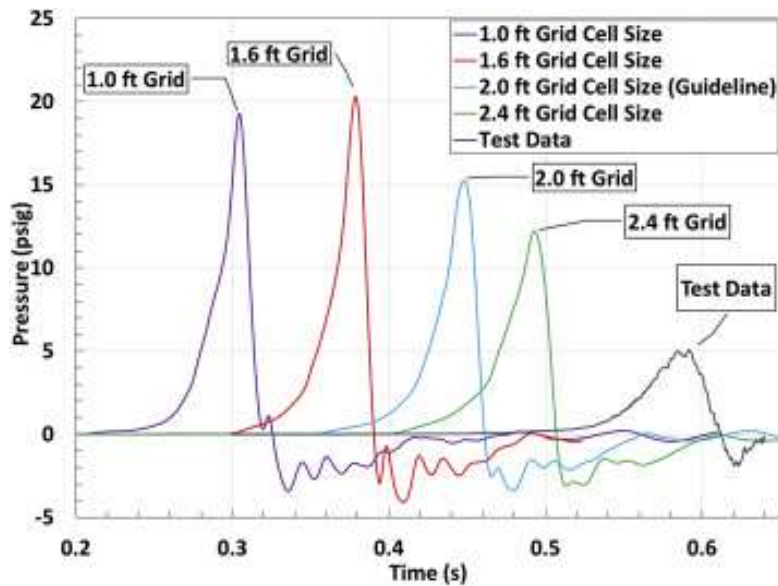
Durán, Goodrich, Kumpukattu-Thomas, Propagation of a Vapor Cloud Detonation from a Congested Into an Uncongested Area, 2012



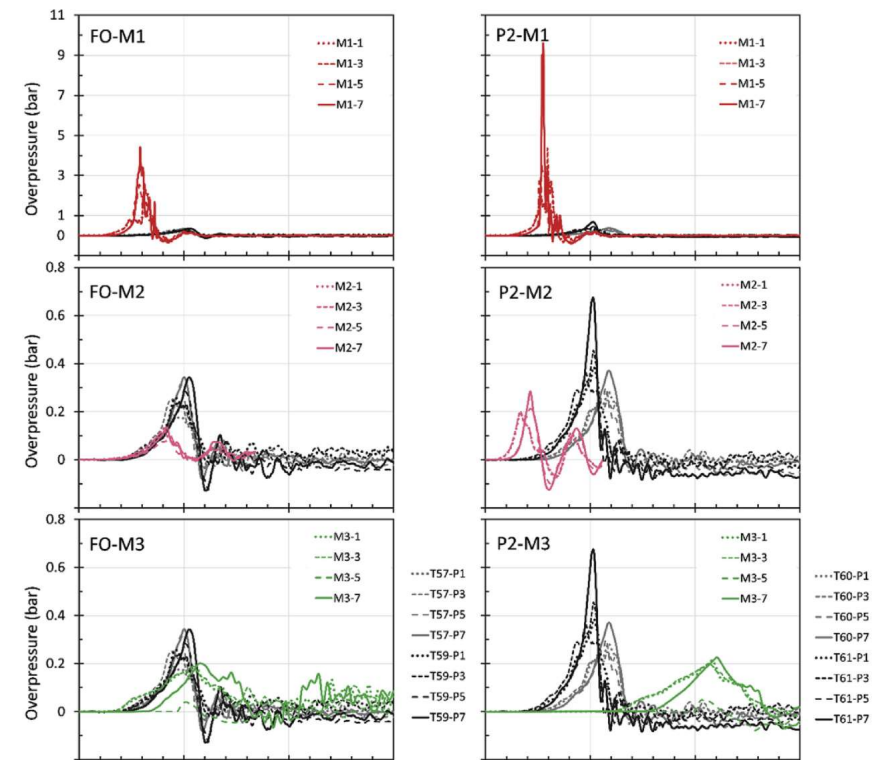
Higher Order Models

FLACS, OpenFOAM/HyFOAM, Converge CFD are examples of CFD codes used for vented deflagration analysis. Grid effects matter.

Vented deflagration experiments performed in 20-foot shipping containers as part of the project Improving hydrogen safety for energy applications through pre-normative research on vented deflagrations (HySEA)



Diakow, Thomas, Vivanco, "Comparison of large-scale vented deflagration tests to CFD simulations for partially congested enclosures", Journal of Loss Prevention in the Process Industries Volume 56, November 2018



Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for inhomogeneous mixtures in 20-foot ISO containers Skjold, 2019

Hazard Analysis & Mitigation



Deflagration venting of a 20' shipping container

Blind-prediction: Estimating the consequences of vented hydrogen deflagrations for inhomogeneous mixtures in 20-foot ISO containers
Skjold, 2019

Engineered Features

Explosion Venting (NFPA 68)

Forced Ventilation (NFPA 69)

Spark and Vent

Passive Ventilation

Sources of Data

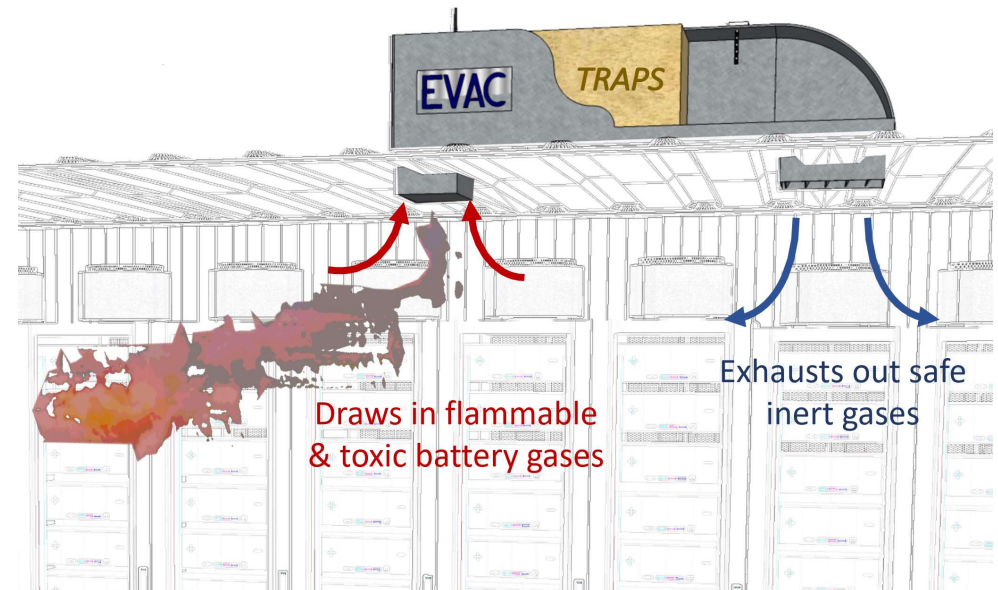
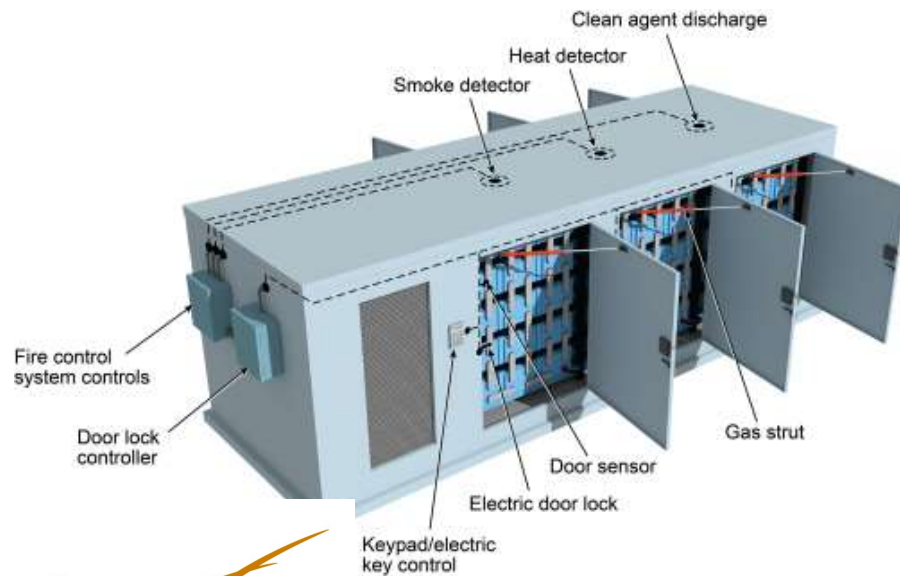
UL 9540A

Peer-reviewed literature

Other testing

Validated models?

New Ideas



Unknowns and Sources of Uncertainty

- How do we model turbulent burning rates?
- How does one model congestion for BESS?
- What benchmark tests and databases do we need?
- How do we model and qualify mitigation measures?
- How do we model partial volume deflagrations?

Summary

Details of gas properties and impact on deflagration modeling have not been considered for gas mixtures representative of battery failures.

Processes for assessing tools for consequence modeling need refinement.

Rational frameworks for coupling data and models for hazard analysis are needed.