Hydrogen and Fuel Cells Program
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State of the art for gaseous release models

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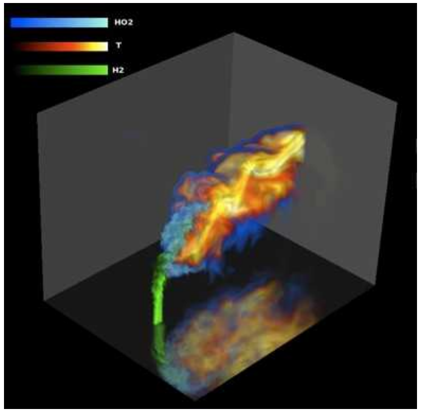
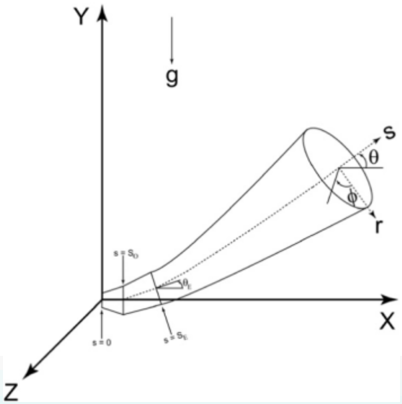
U.S. DEPARTMENT OF ENERGY

Models vary in terms of computational resources required, resolution, and fidelity

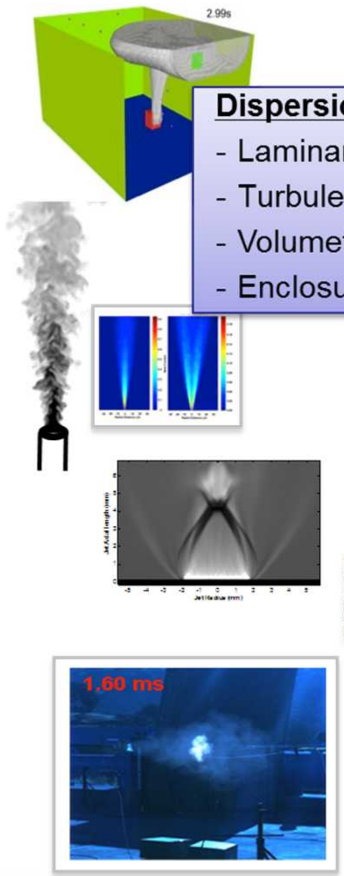
- Computational Fluid Dynamics
  - DNS, LES, RANS
  - dimensions (symmetry?)
  - transient vs. steady-state
  - chemistry
- Reduced order models
  - limit to centerline coordinate (1-D)
  - assume profile around centerline coordinate
- **All models require validation**
  - validation data accuracy
  - boundary conditions
  - range of use



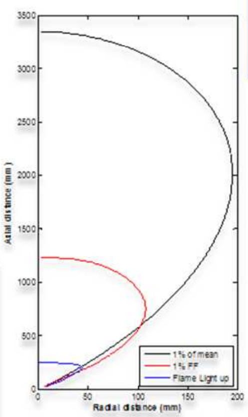
http://www.princeton.edu/cefrc/Files/2012%20Lecture%20Notes/Chen/Princeton-CEFRC-Summer-School-Chen2.pdf



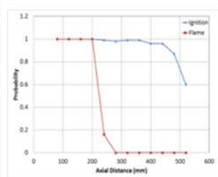
We focus on validated reduced-order models that can inform risk models

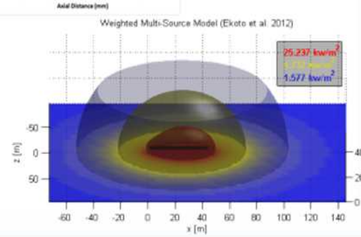


Dispersion Characteristics
- Laminar Flow
- Turbulent jet
- Volumetric rupture
- Enclosure Accumulation



Ignition Probability
- Ignition mechanism
- Mixture ignitability
- Ignition delay/location
- Sustained light-up





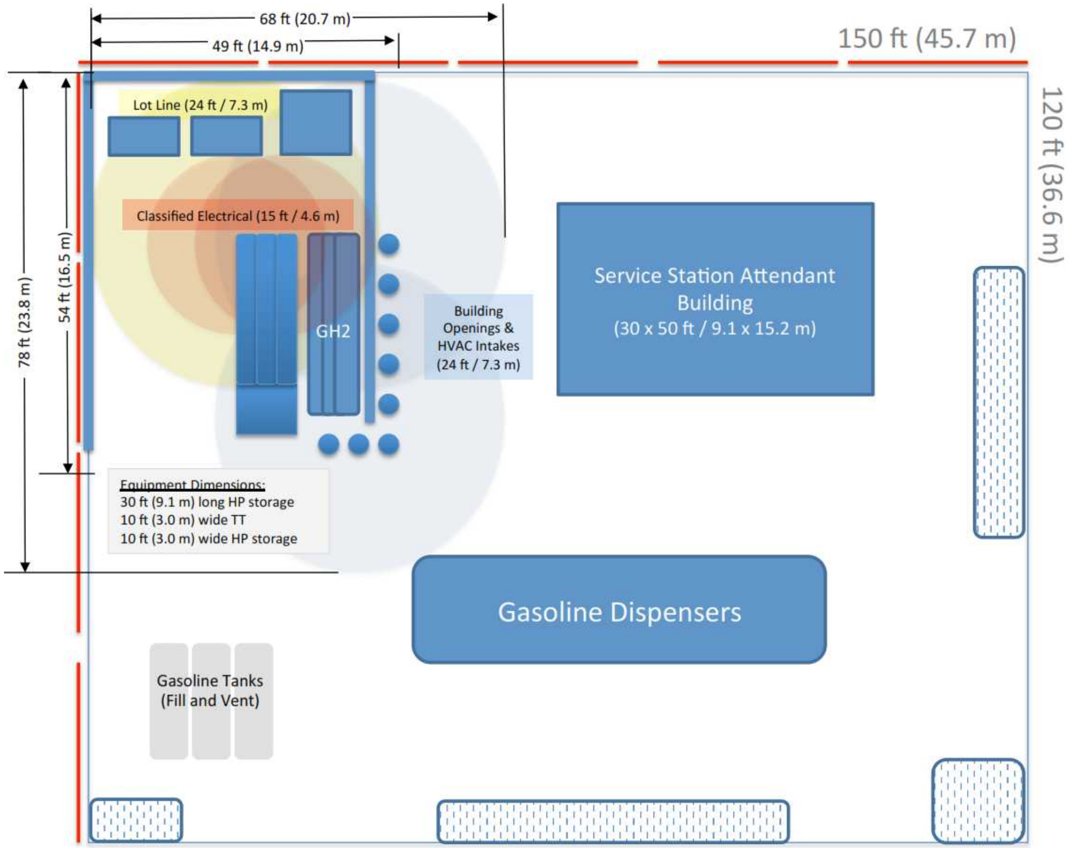
Hazard Characteristics
- Flame radiation
- Overpressure (deflagration/detonation)
- O_2 dilution/depletion

Risk requires a **Release**, then **Ignition**, forming a **Hazard**, causing **Harm**

- We ***quantify*** each of these events using models
- **Purple** events quantified with statistical models, **Red** with reduced-order behavior models

Our goals are to quantitatively model the release and hazard behaviors

Feature	distance ft (m)
Lot lines	24 (7.3)
Public streets, alleys	24 (7.3)
Parking (public assembly)	13 (4.0)
Buildings (sprinklers, fire rated)	10 (3.0)
Building openings or air intakes	24 (7.3)
Flammable and combustible liquid storage, vents or fill ports	10 (3.0)
Parking from fill concentrations on bulk storage	13 (4.0)
Class 1 Division 2 area diameter	15 (4.6)

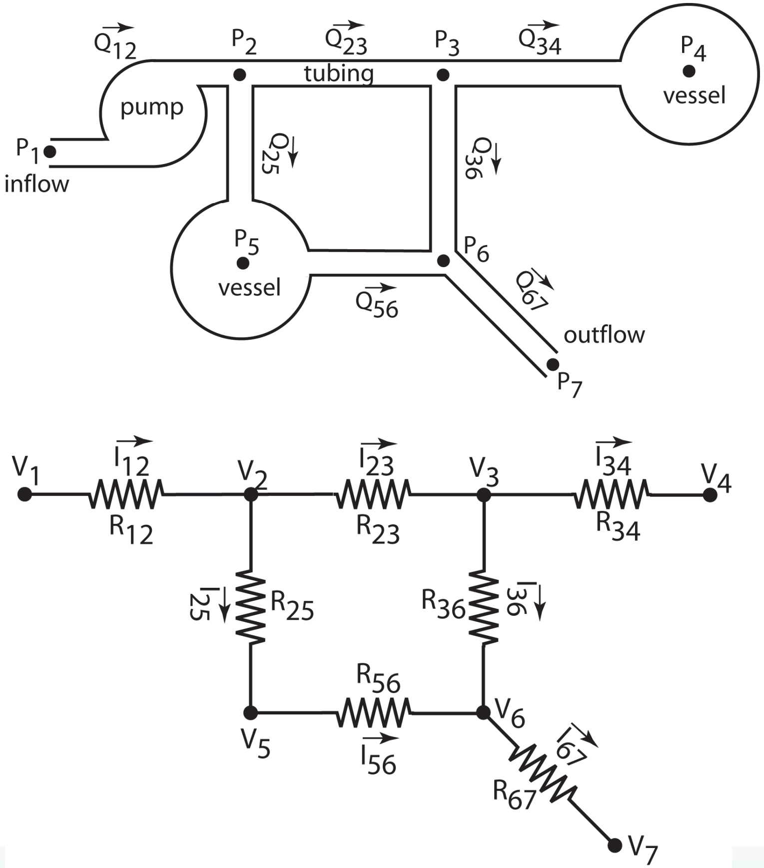


Harris et al., SAND2014-3416

- what are the hazards?
- are these distances appropriate?

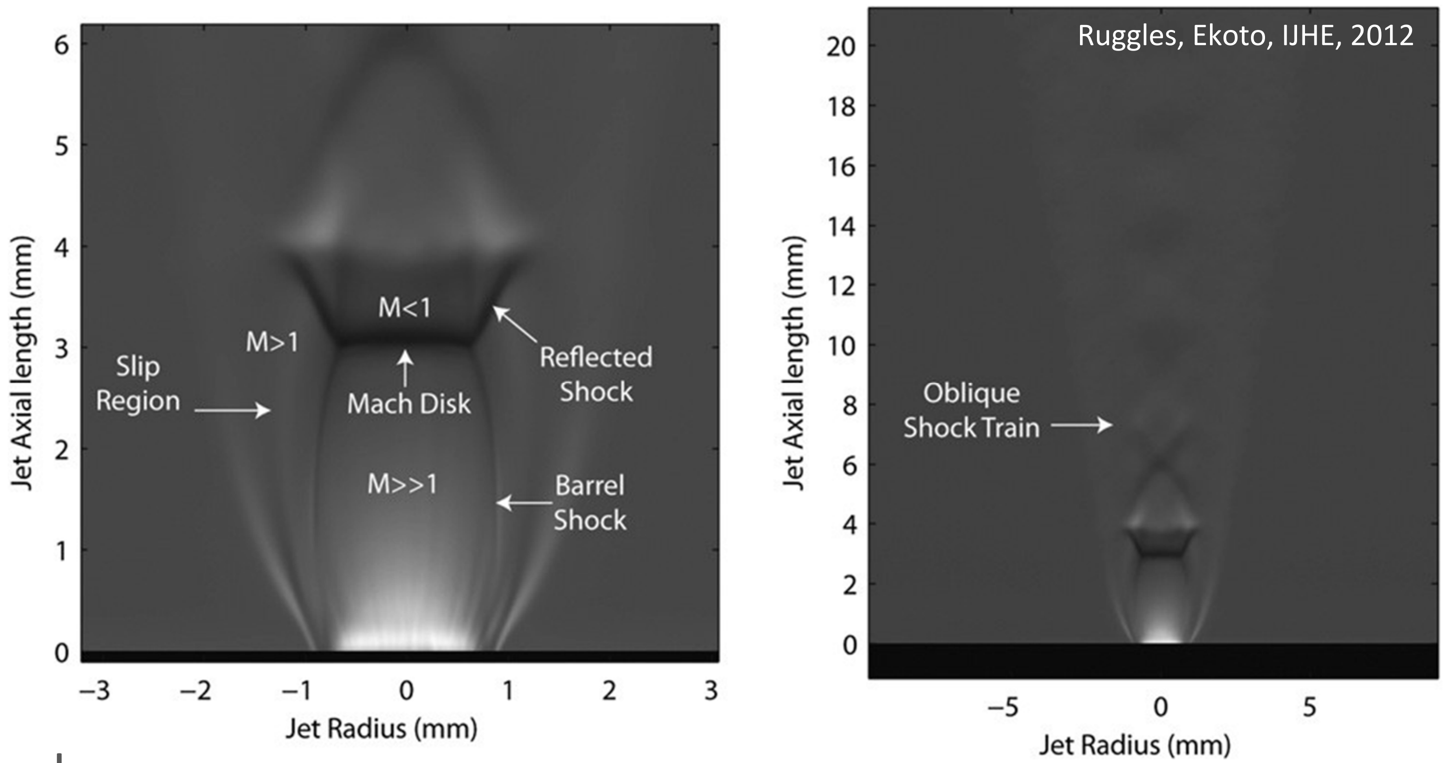
Internal flows can be effectively modeled using a network flow model (NETFLOW)

- 1-D conservation equations solved for an ‘electrical’ network
- nonlinear ‘resistors’ account for flow friction
- ‘voltages’ (pressures) are functions of temperature and composition
- any component with a known relationship between pressure drop and flow can be modeled
- currently only for compressible gas flows



SAND2001-8422

Choked flow can develop from high-pressure sources



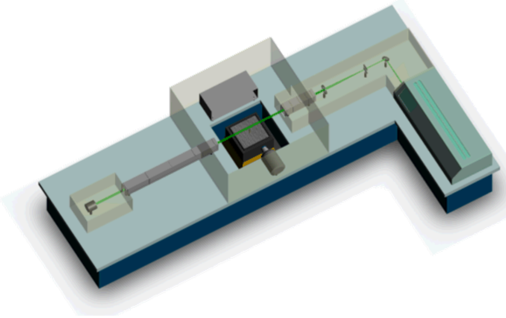
Approach:

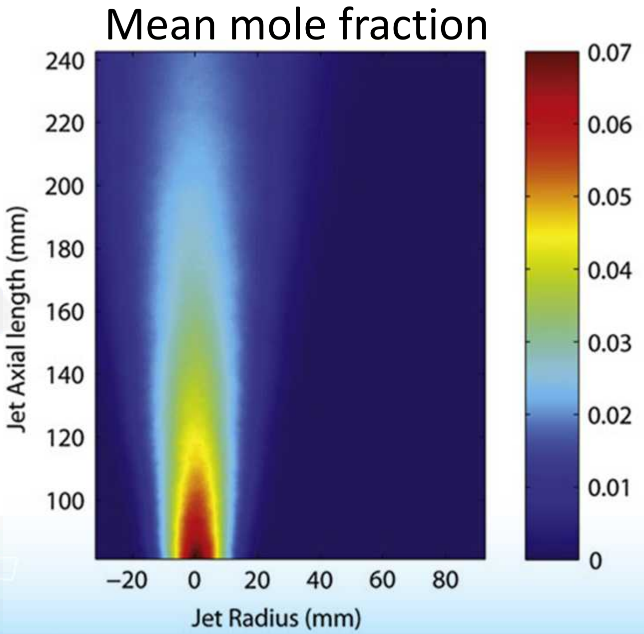
- Notional nozzle to describe effective velocity, diameter, thermodynamic state downstream of the shock structure

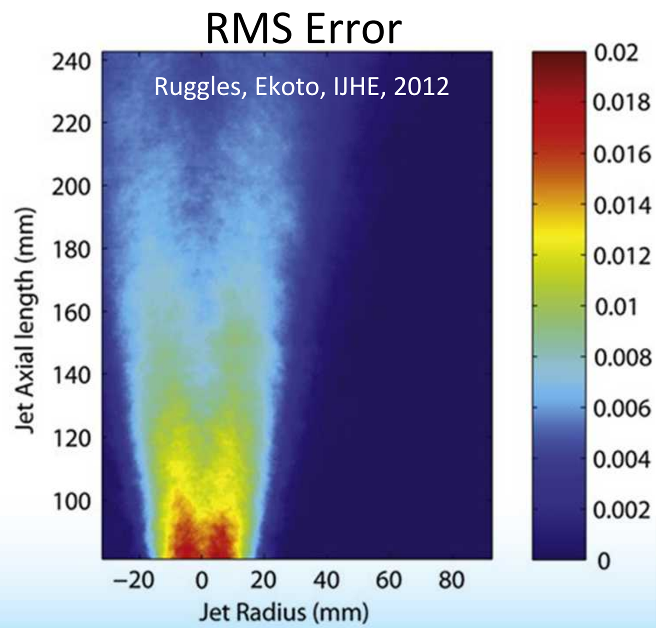
Data is needed for a validated notional nozzle model

Approach:

- Use non-intrusive diagnostics (Rayleigh scattering, Schleren imaging) to quantify jet spreading and flow structure
- Fit model that includes fluid flow across shock and in slip region (with accurate state modeling)

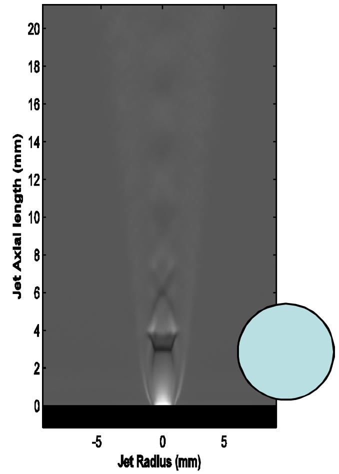






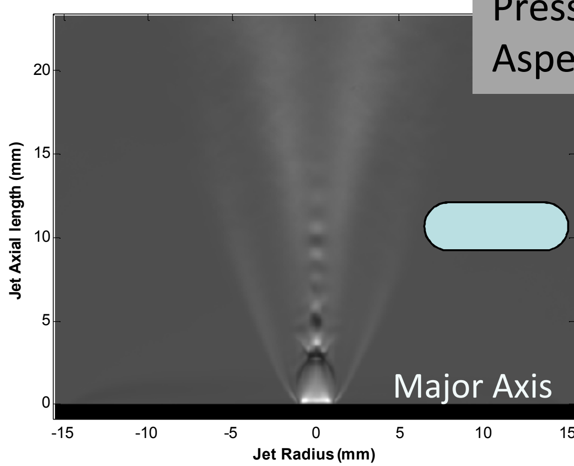
Releases from non-circular orifices show that the jet spreads fastest along the minor axis

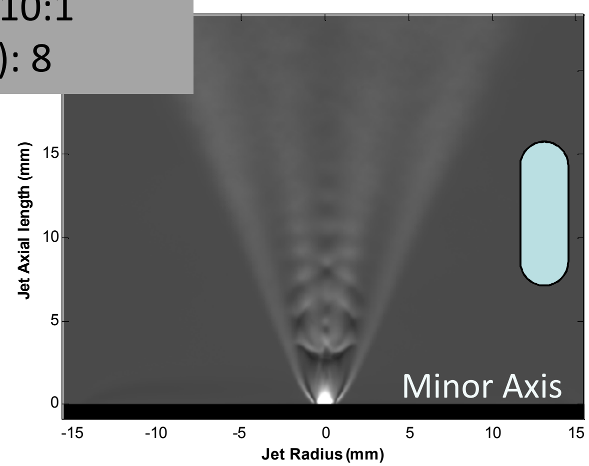
Schlieren images of jet exit shock structure



Pressure Ratio = 10:1
Aspect Ratio (AR): 1

Pressure Ratio = 10:1
Aspect Ratio (AR): 8

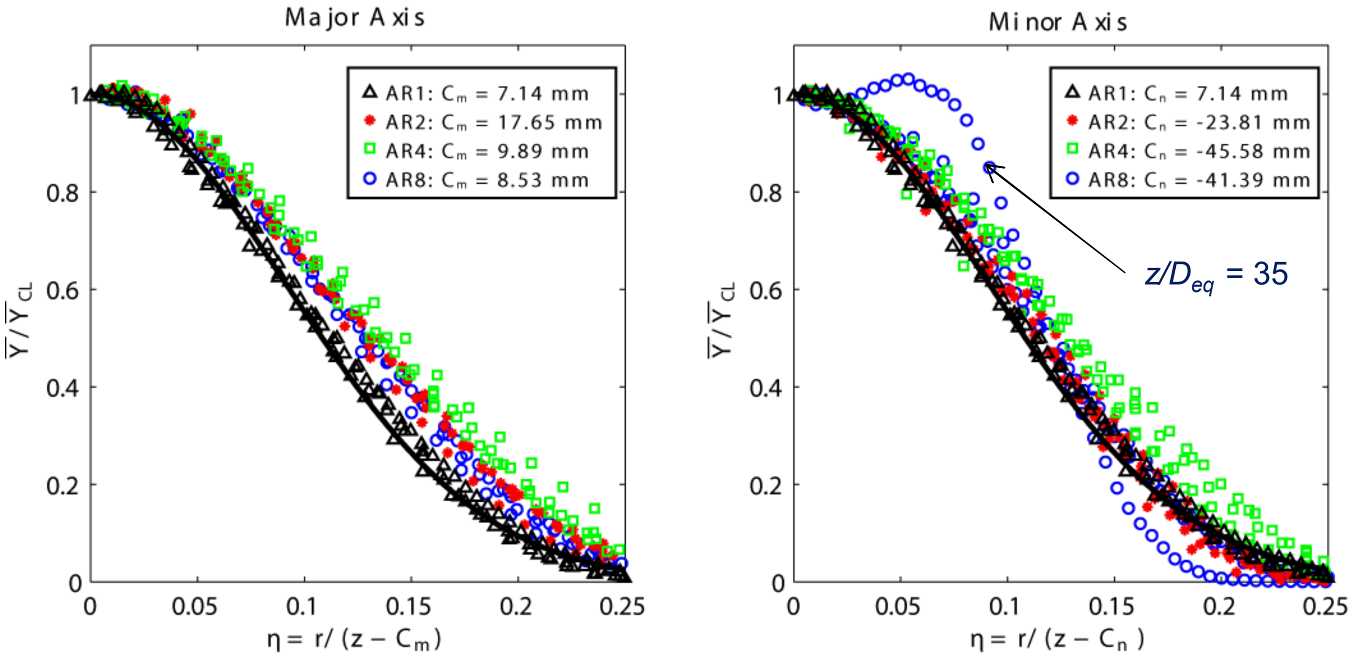




Ruggles, Ekoto, IJHE, 2014

Jet profiles collapse to a single curve far from nozzle

Collapsed profiles deviated from the axisymmetric values and were no longer Gaussian



z/D_{eq} = 35, 69, 102, 136 & 161

Results suggest it should be possible to develop a modified slot jet integral model — remains unclear for lager storage pressures & aspect ratios

Ruggles, Ekoto, IJHE, 2014

A 1-D plume model can describe 3-D flow (in cross-wind) after profile becomes fully developed

assumption: fully-developed velocity & concentration profiles are Gaussian

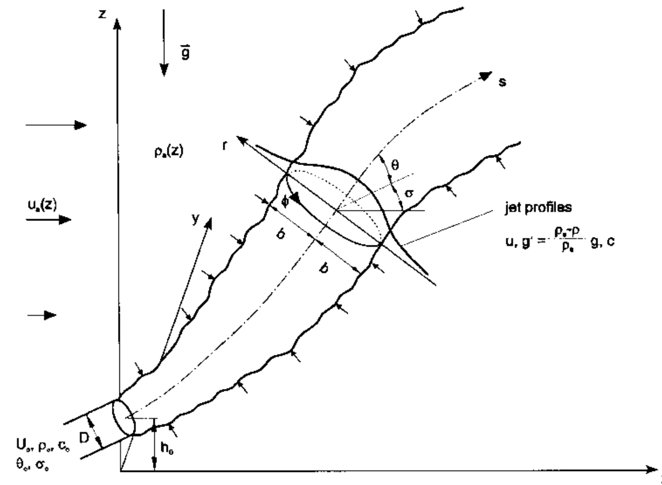
B: velocity jet width

λ: concentration-to-velocity jet width ratio

$$\frac{V}{V_{CL}} = \exp\left(-\frac{r^2}{B^2}\right)$$

$$\frac{\rho - \rho_{amb}}{\rho_{CL} - \rho_{amb}} = \exp\left(-\frac{r^2}{\lambda^2 B^2}\right)$$

$$\frac{\rho Y}{\rho_{CL} Y_{CL}} = \exp\left(-\frac{r^2}{\lambda^2 B^2}\right)$$



parameters based on empirical data

Mass $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} \rho V r\,dr\,d\phi = \rho_{amb} E$$

x-Mom $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} \rho V^2 \cos\theta \sin\sigma\, r\,dr\,d\phi = -F_D \frac{\cos^2\theta \sin\sigma \cos\sigma}{\sqrt{1-\cos^2\theta\cos^2\sigma}}$$

y-Mom $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} \rho V^2 \cos\theta \cos\sigma\, r\,dr\,d\phi = U_{wind} E \rho_{amb} + F_D\sqrt{1-\cos^2\theta\cos^2\sigma}$$

z-Mom $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} \rho V^2 \sin\theta\, r\,dr\,d\phi = \int_0^{2\pi}\int_0^{\infty} (\rho_{amb}-\rho) g r\,dr\,\phi - F_D \frac{\sin\theta\cos\theta\cos\sigma}{\sqrt{1-\cos^2\theta\cos^2\sigma}}$$

Species $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} c V r\,dr\,d\phi = 0$$

Energy $$\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty} \rho V (h - h_{amb}) r\,dr\,d\phi = 0$$

$$\frac{dx}{dS} = \cos\theta\cos\sigma$$

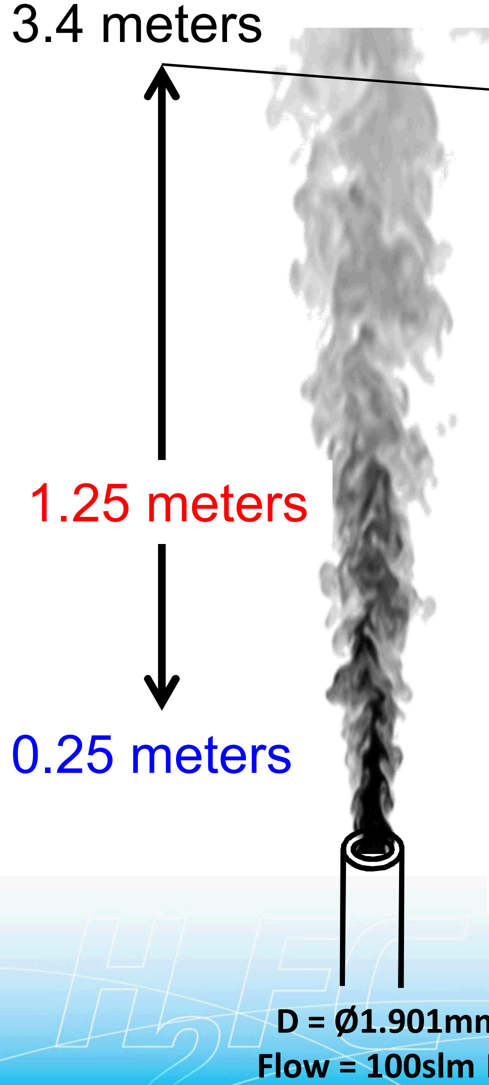
$$\frac{dy}{dS} = \cos\theta\sin\sigma$$

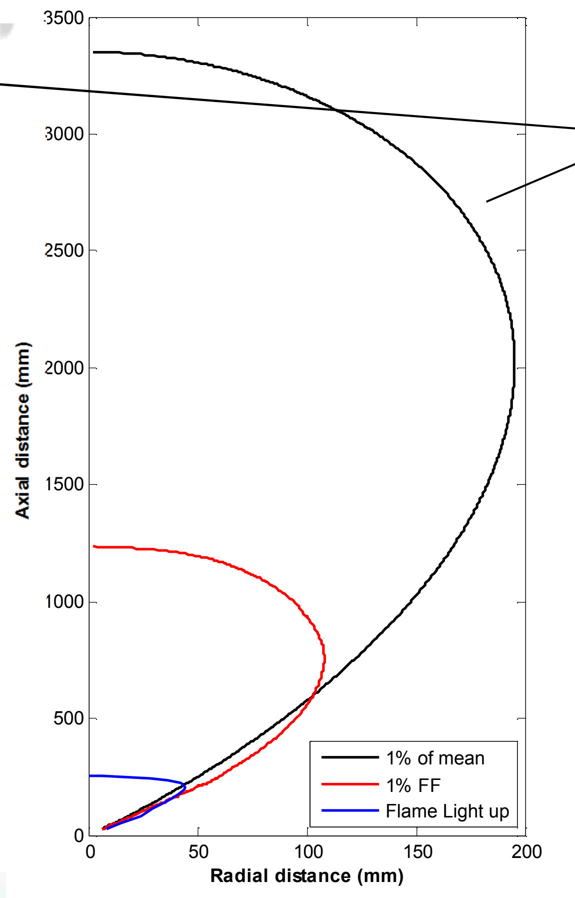
$$\frac{dz}{dS} = \sin\theta$$

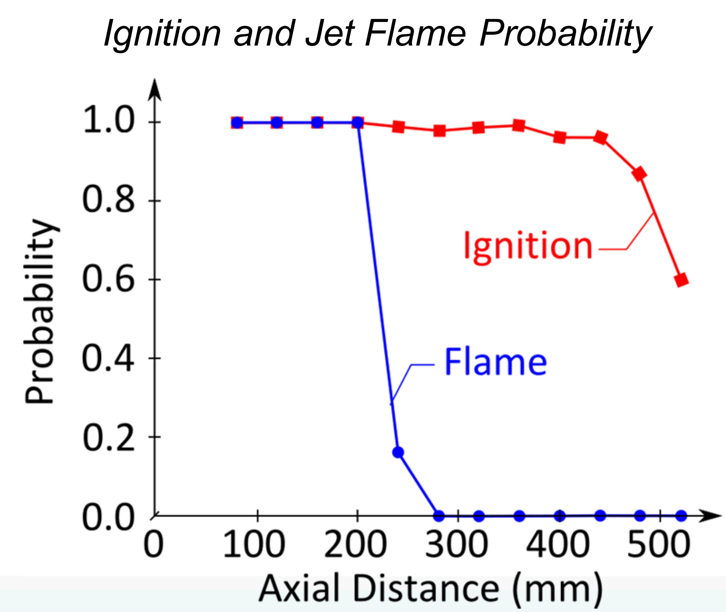
- map out flammable extents
- determine concentration at building inlets

Jirka, EFM, 2004

Flammability factor provides sound basis for identifying jet flame ignition boundaries





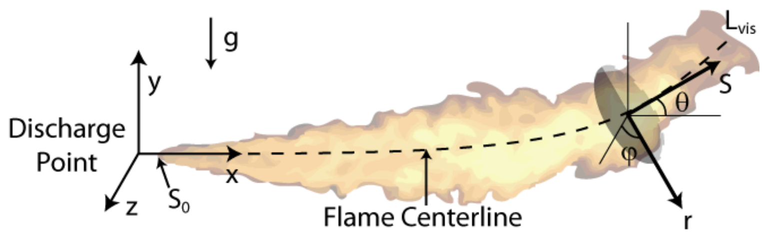


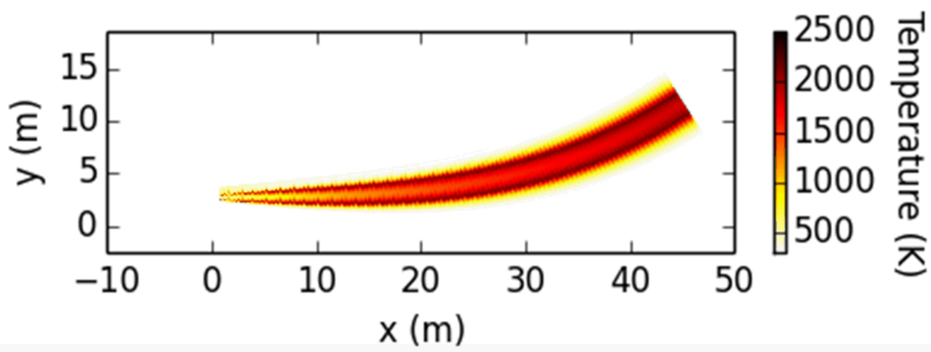
Provides pathway for reduced separation distances

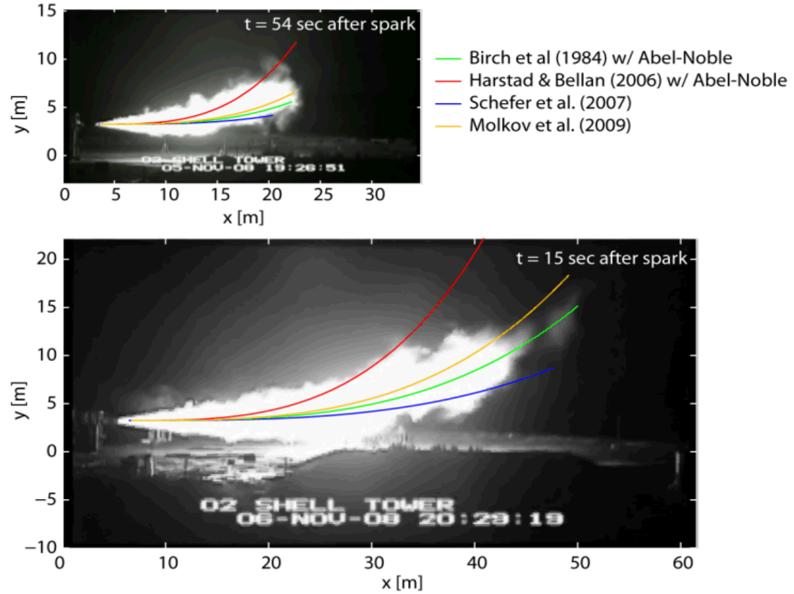
A 1-D flame model can describe 3-D flames, including buoyancy and wind

$$\underbrace{\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty}\rho V Y r dr d\phi}_{\text{species conservation}} \text{ replaced by, } \underbrace{\frac{d}{dS}\int_0^{2\pi}\int_0^{\infty}\rho V f r dr d\phi}_{\text{mixture fraction conservation}}$$

where, $f = Y_{H_2} + Y_{H_2O}\frac{MW_{H_2}}{MW_{H_2O}}$





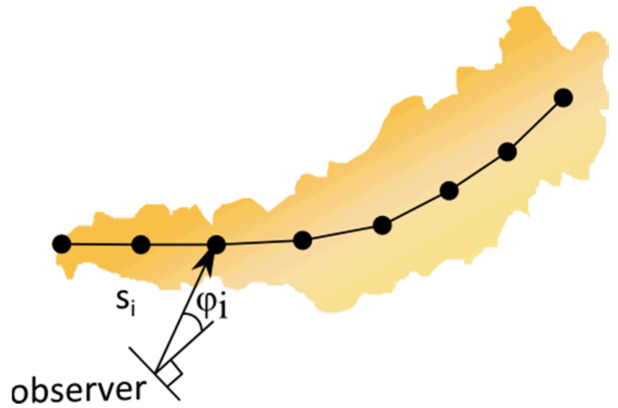


Ekoto et al. ICHS, 2012

- Results highly dependent on boundary conditions (notional nozzle formulation)

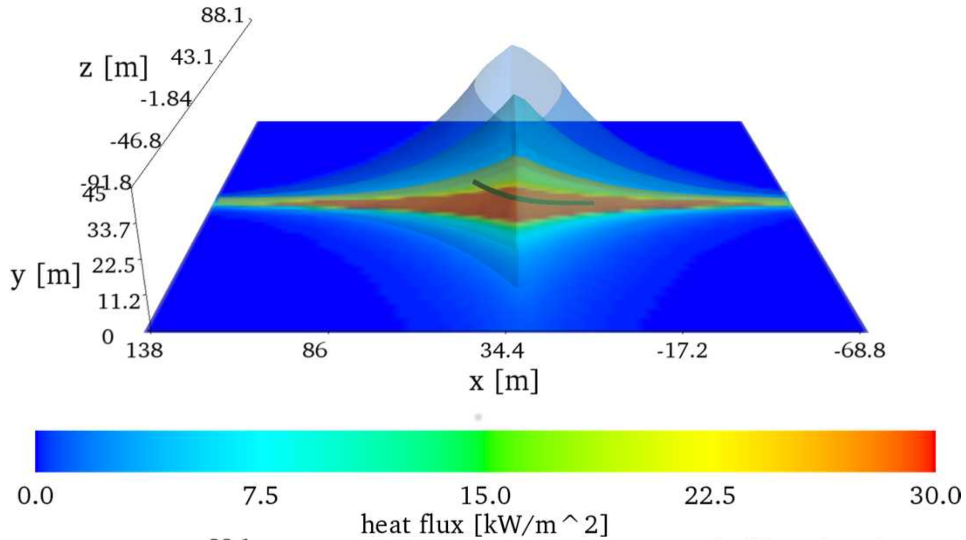
A multi-source radiation model can account for variable flame width and curvature

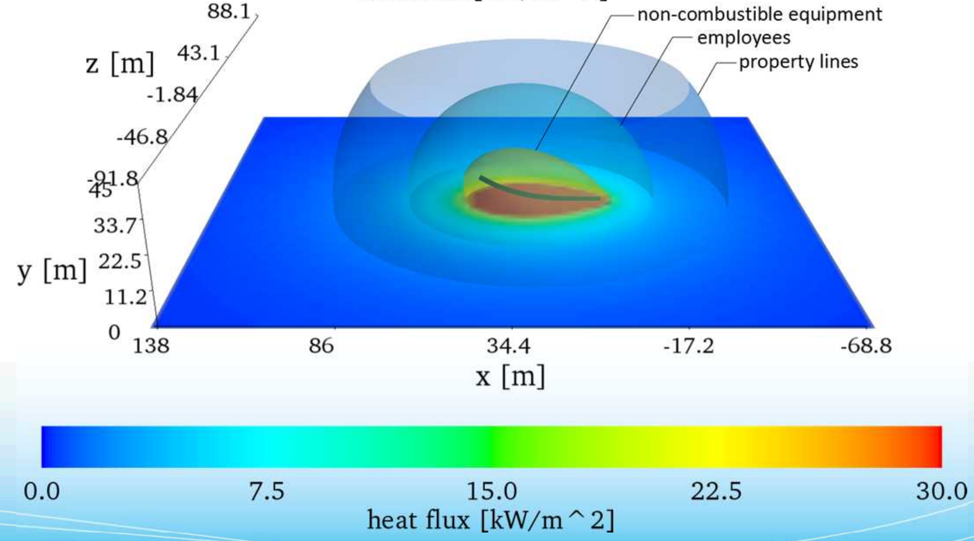
Hankinson & Lowesmith, Comb & Flame, 2012



- identify heat-flux hazard boundaries
- no large standoff distances normal to center of flame

Ekoto et al. ICHS, 2012





Walls reduce the hazards and change plume shape, but reduced-order models require development

Possible to:

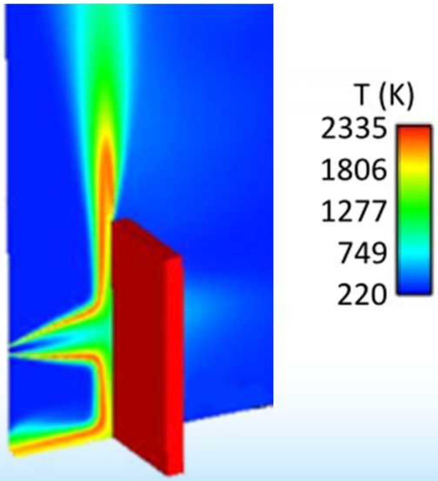
- reduce extent of flammable cloud
- deflect jet flames
- reduce magnitude of radiative heat flux
- minimize ignition overpressure

But necessary to consider:

- reflection of radiative heat flux
- flammable concentrations can increase in some areas

Is it possible to reduce the dimensionality with self similar solutions?

Schefer et al., IJHE, 2009



Houf et al., IJHE, 2009

The buoyancy of hydrogen often causes stratified mixtures to form

- accumulation in ceiling layer
- ventilation can cause mixing
- hydrogen can be drawn in vents (importance of plume modeling)

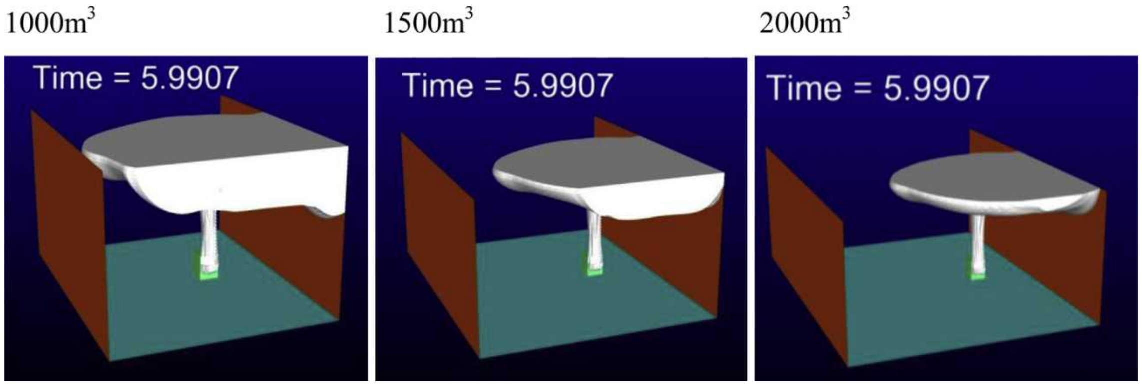
layer volume:

$$\frac{dV_{\text{layer}}}{dt} = Q_{\text{jet}} - Q_{\text{out}}$$

layer concentration:

$$V_{\text{layer}}\frac{dc}{dt} = Q_{\text{H}_2}(1-c) - cQ_{\text{air}}$$

Lowesmith et al., IJHE, 2009

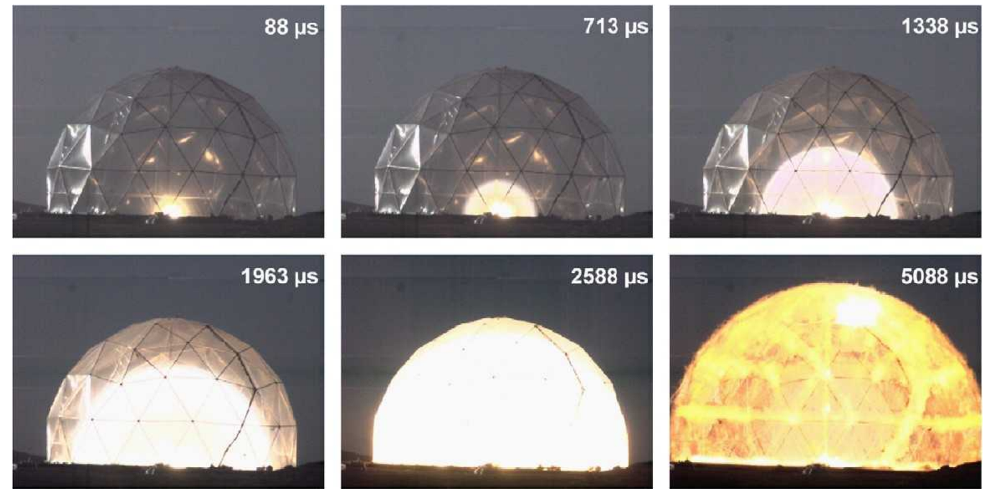


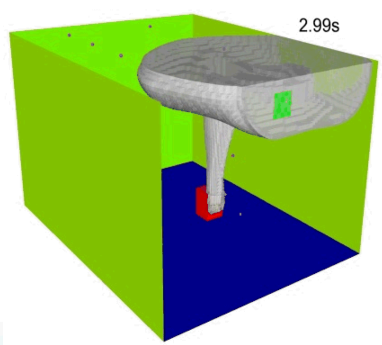
Houf et al., IJHE, 2012

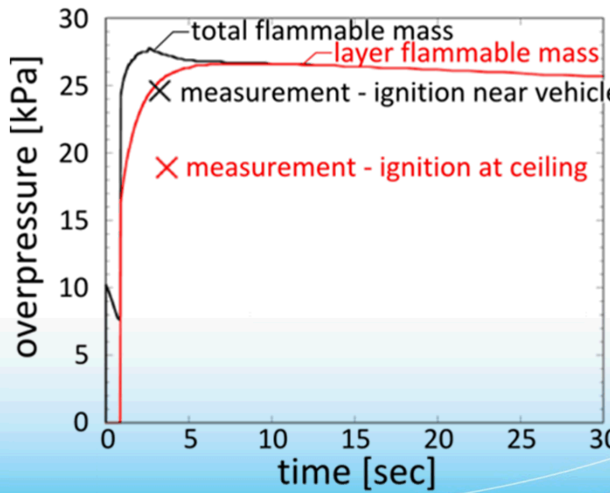
Ignition of an accumulated mixture can cause a significant overpressure hazard

- CFD can effectively model complex configurations
- Reduced order models need to consider effects from:
  - flame instabilities
  - obstacles
  - stratified mixtures
  - volumetric venting
- external ignition reduced-order overpressure model needs development

Groethe et al., IJHE 2007







$$\Delta p = p_0 \left[\left(\left(\frac{V_T + V_{H_2}}{V_T} \right) \left(\frac{V_T + V_{\text{stoich}}(\sigma - 1)}{V_T} \right) \right)^{\gamma} - 1 \right]$$

Bauwens & Dorofeev, ICHS, 2014.

Summary

Effective reduced-order models:

- plume
- flammability limits
- flame
- multi-source radiation
- accumulation/layer
- overpressure

Research needs:

- incompressible/phase-change network flow
- notional nozzle model
- non-circular orifice
- walls/barriers
  - pressure
  - radiation
- non-enclosed overpressure
- transient effects

- **Validation data over a wide range of conditions, with clearly defined boundary conditions**

Acknowledgements

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