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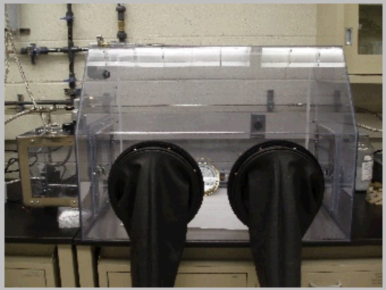

Closed Vessel Deflagrations and Resulting Overpressures

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U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Introduction

- Reasons for Performing Analysis
- Computer Based Models
- TNT Method
- Closed Vessel (Cooper's Methodology)
- Example
- Detonation
- Deflagration-to-Detonation Transition
- Questions

Title page – left photo: U.S. CSB. 2011. Bayer CropScience Pesticide Waste Explosion, Retrieved from http://www.csb.gov/bayer-cropscience-investigative-photos-/

Title page – left photo: U.S. CSB. 2011. Williams Olefins Plant Explosion, Retrieved from http://www.csb.gov/williams-olefins-incident/

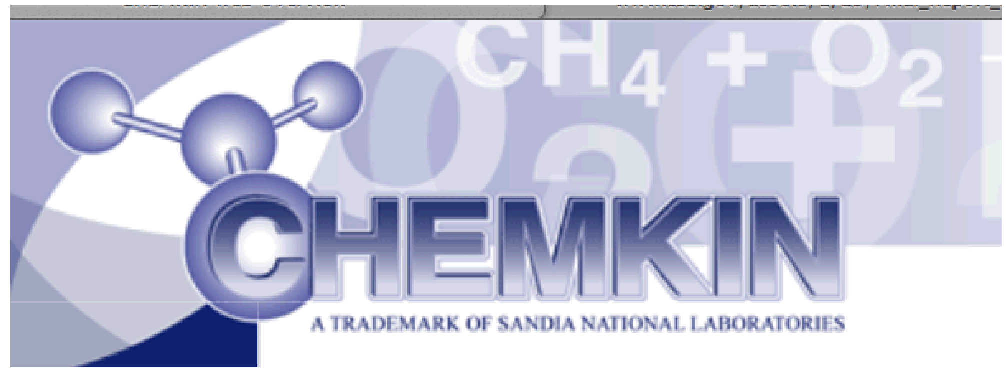
Reasons for Performing

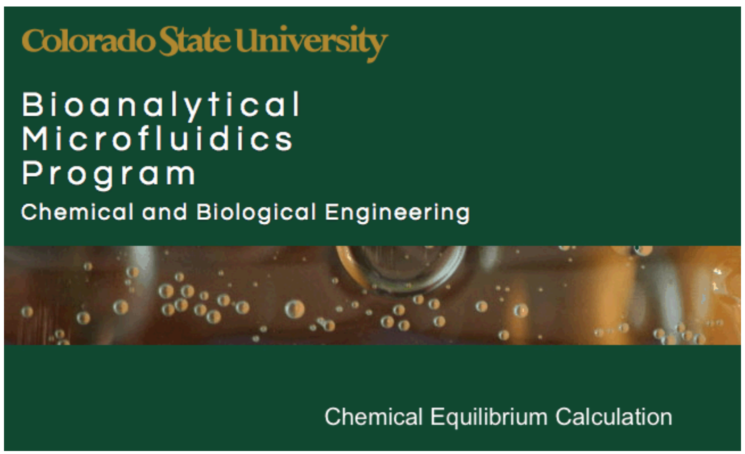
- Internal deflagrations involving flammable gases/vapors/dust
  - Natural gas leak in a CUB
  - Processes involving flammable gas mixtures
  - Impacts of unmitigated scenarios
  - Accident investigation
- Facility/Equipment Design
- Deflagration Detonation Transitions

U.S. CSB. 2008. Imperial Sugar Investigative Photos, Retrieved from http://www.csb.gov/imperial-sugar-investigative-photos/

Computer Based Models

- STANJAN – no longer supported
- Commercial CFD packages
- HPFLAME
- UVFLAME





Safety Software
DOE O 414.1D/ASME NQA-1
verification – validation – inventory – configuration management – documented training

TNT Method

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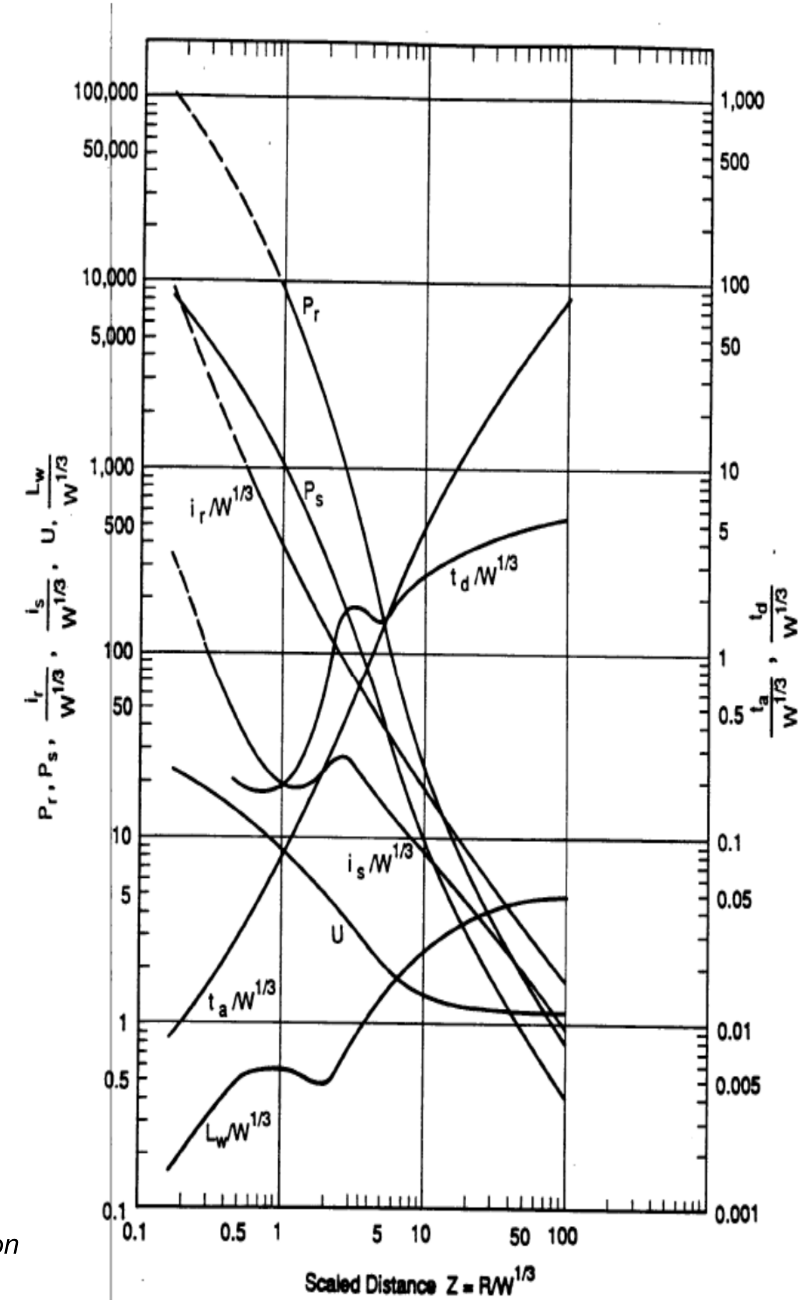
$$m_{TNT} = \frac{\eta m \Delta H_c}{E_{TNT}}$$

Where

m_{TNT}	= equivalent mass of TNT
η	= empirical explosion efficiency (unitless)
m	= mass of hydrocarbon
ΔH_c	= combustion or energy of explosion
E_{TNT}	= is the energy of explosion of TNT

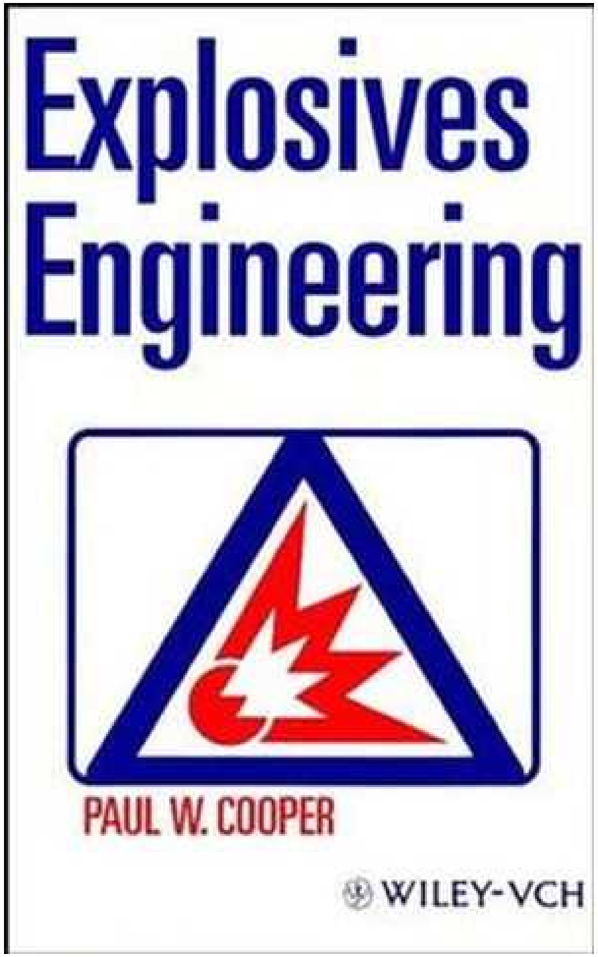
Empirical explosion efficiency is one of major problems for method. Reported values range from 1 to 15%.

Only considers explosion



U.S Department of Energy (July 1992). *A Manual for the Prediction of Blast and Fragment Loadings on Structures.* DOE/TIC-11268

Closed Vessel Overpressure



- Cooper provides a great description/example
- SFPE Handbook 4th Edition
  - Expands on impulse
- Simple analysis to perform
  - Adiabatic flame temperature
  - Find static pressure
    - Ideal gas law
      - Flame temperature
      - Moles of product
  - Adjust pressure for constant volume constraint

Example

- Problem
  - Propane gas fills fume hood that lost its ventilation
  - Assumptions
    - 48 in. w x 36 in. d x 59 in. h
    - Ambient Temp = 20 C
    - Ambient Pressure = 1 atm
    - Propane (C_3H_8)
      - MW = 44 g/mol
      - ΔHc = 620 kcal/mol
      - LFL = 2.1%
- Determine Hood Volume – 1.67m^3

Labconco. 2014. 4’ Protector XStream Laboratory Hood
http://www.labconco.com/product/4-protector-xstream-laboratory-hood-5/3748

Example (continued)

- Propane is at LFL
- Moles of gas

$$n_{gas} = \frac{PV}{RT} = 70$$

- Moles of constituents

$$n_{C_3H_8} = 0.021 n_{gas} = 1.5$$

$$n_{air} = n_{gas} - n_{C_3H_8} = 68.5$$

$$n_{O_2} = 0.21 n_{air} = 14.4$$

$$n_{N_2} = 0.79 n_{air} = 54.1$$

- Chemical balance

$$1.5C_3H_8 + 14.4O_2 + 54.1N_2 \longrightarrow 4.5CO_2 + 6H_2O + 6.9O_2 + 54.1N_2$$

- Total moles after reaction = 71.5

Example (continued)

- Temperature of the gases

Heat produced = Heat absorbed by products $$Q = n\int_{T_0}^{T_a} C_p \, dT$$

Heat produced $$Q = (1.5mol)\left(530.6\, {kcal}/{mol}\right) = 796kcal$$

Specific heat is a function of temperature

$$C_p = a + bT + cT^2$$

$$\bar{a} = \sum_i n_i a_i$$

$$x_{CO_2} = {4.5}/{71.5} = 0.063$$

$$x_{H_2O} = {6}/{71.5} = 0.084$$

$$x_{O_2} = {6.9}/{71.5} = 0.100$$

$$x_{N_2} = {54.1}/{71.5} = 0.76$$

Example (continued)

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Table 8.2 Empirical constants for molal heat capacities of gases at constant pressure ($p = 0$) $C_p = a + bT + cT^2$, where T is in degrees Kelvin; (g cal) / (g mole) (K); temperature range 300 to 1500 K

Gas	a	$b(10^3)$	$c(10^6)$
H_2	6.946	−0.196	+0.4757
N_2	6.457	1.389	−0.069
O_2	6.117	3.167	−1.005
CO	6.350	1.811	−0.2675
NO	6.440	2.069	−0.4206
H_2O	7.136	2.640	+0.0459
CO_2	6.339	10.14	−3.415
SO_2	6.945	10.01	−3.794
SO_3	7.454	19.13	−6.628
HCl	6.734	0.431	+0.3613
C_2H_6	2.322	38.04	−10.97
CH_4	3.204	18.41	−4.48
C_2H_4	3.019	28.21	−8.537
Cl_2	7.653	2.221	−0.8733
Air	6.386	1.762	−0.2656
NH_3^a	5.92	8.963	−1.764

Cooper, P.W. (1996). *Explosives Engineering,* ISBN *0-471-1836-8,* Wiley-VCH

Example (Continued)

- Temperature of the gases (continued)

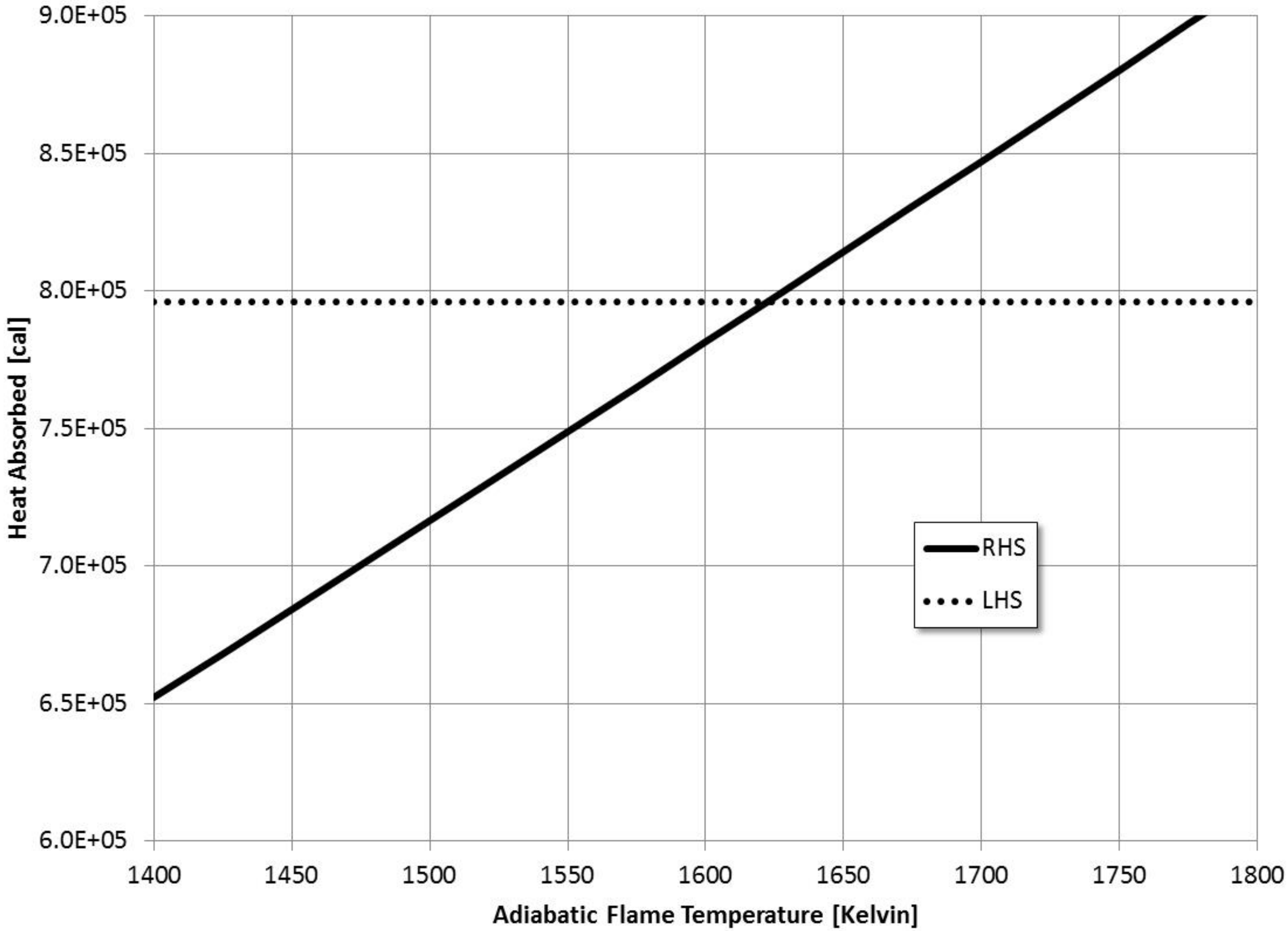
$$Q = n\int_{T_0}^{T_a}\left(6.517 + 2.2333\times10^{-3}T - 3.642\times10^{-7}T^2\right)dT$$

$$Q = n\left[6.517\left(T_a - T_0\right) + \frac{2.233\times10^{-3}}{2}\left(T_a^2 - T_0^2\right) - \frac{3.642\times10^{-7}}{3}\left(T_a^3 - T_0^3\right)\right]$$

How to solve??

Example Continued

- Temperature of the gases (continued)



Example (continued)

- Deflagration Pressure

$$P_D = \frac{nRT}{V} = \frac{(71.5mol)\left(8.314\, {}^{J}\!/_{mol \cdot K}\right)(1625K)}{1.67m^3}$$

$$P_D = 578.4kPa$$

Correct for constant volume condition – ratio of specific heats

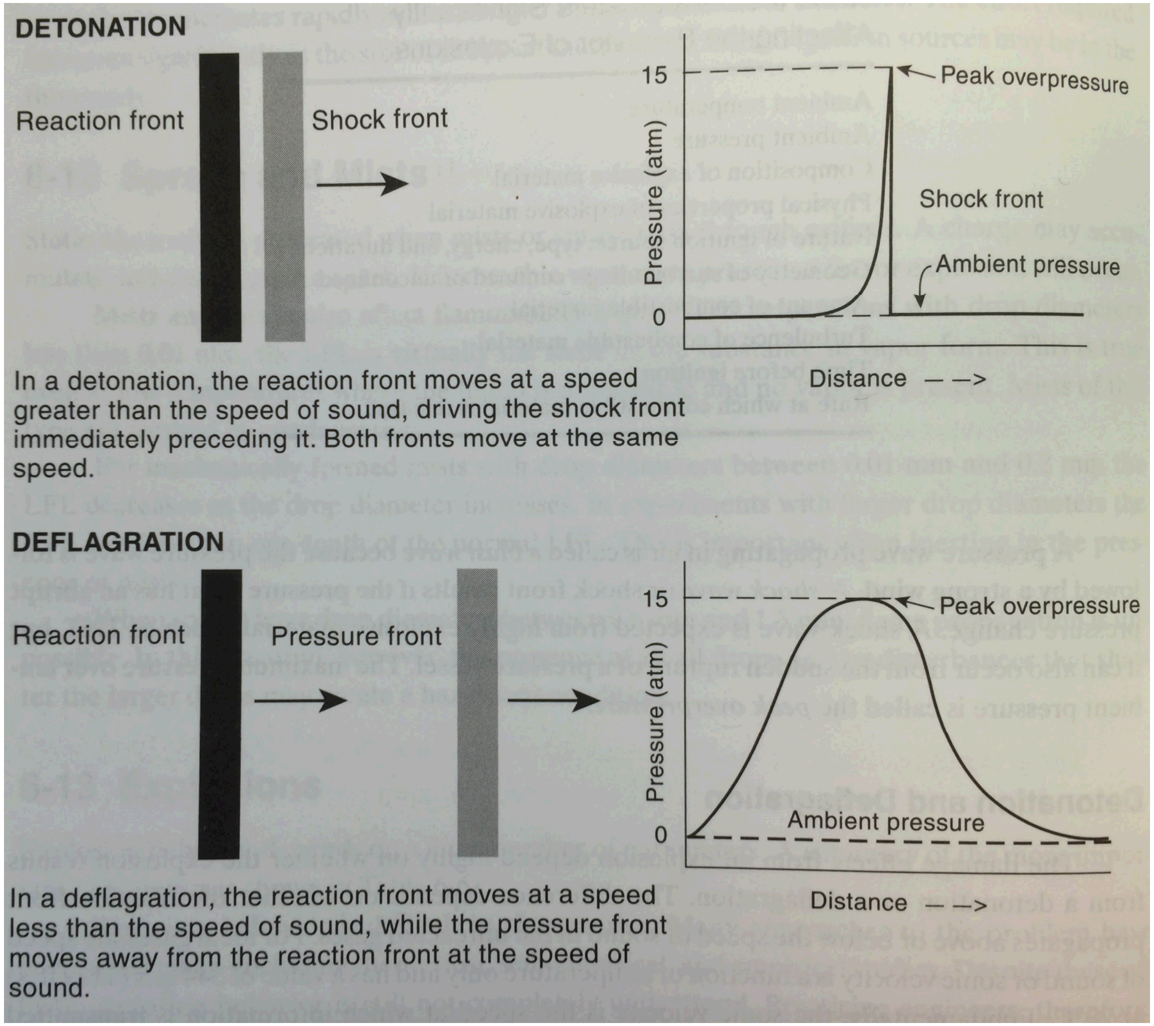
$$P_{\max} = \gamma P_D$$

$$\bar{\gamma} = \sum_i x_i \gamma_i$$

$$P_{\max} = 1.4(578.4kPa) = 809.8kPa$$

Detonation

- Chapman-Jouguet (C-J) Pressure ~ 2Pmax
  - SFPE Handbook
- Reflected shock ~2.76$P_{C\text{-}J}$
- Rough estimates



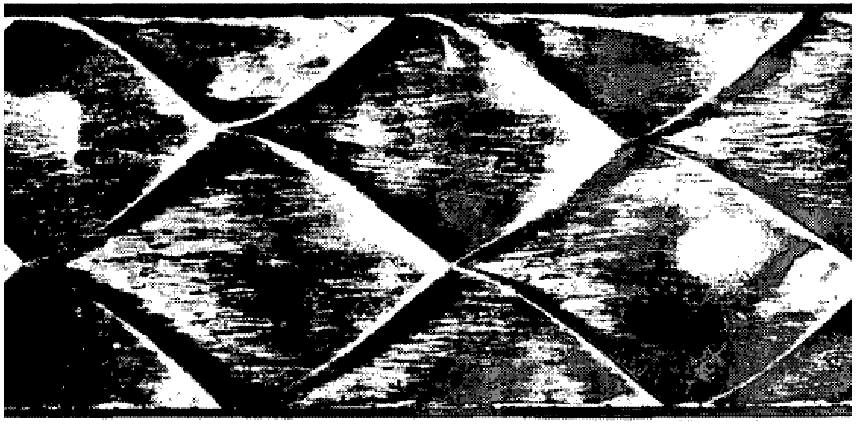
Crowl, D.A., and Louvar, J.F. (2002). *Chemical Process Safety: Fundamentals with Applications.* Prentice-Hall

Deflagration-to-Detonation Transition

- Depends on
  - Mixture reactivity
  - Enclosure roughness/obstructions
  - Pipes – Sc/3
  - Open pipe end – 13Sc

for Stoichiometric Gas-Air Mixtures

Gas	C-J Mach Number	Cell Width (cm)[21]
Acetylene	5.46	0.98
n-Butane	—	5.0–6.2
Ethane	—	5.4–6.2
Ethylene	—	2.8
Hydrogen	4.89	1.5
Hydrogen sulfide	—	10
Methane	5.17	28
Propane	5.38	6.9
Propylene	—	5.4



Top: Zalosh, R (2008). *Explosion Protection*. SFPE Handbook of Fire Protection Engineering, Society of Fire Protection Engineers, Bethesda, MD

Bottom: Tieszen, S.R., et. al. (1987). *Detonability of H2-Air-Diluent Mixtures,* NUREG/CR-4905, U.S. Nuclear Regulatory Commission

Questions