

# The Modeling of LNG Spreading on Water

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June 12, 2007

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company,  
for the United States Department of Energy under contract DE-AC04-94AL85000.

# Factors Affecting Spreading

**Classified as a multi-phase, multi-component problem. Very complicated with several factors affecting pool spread dynamics:**

- **Geometric considerations**
  - Unconfined or confined
  - Surrounding structures
  - Depth of water
  - Height of release
- **Composition**
- **Rapid phase transitions**
- **Waves, currents, and wind**
- **Pool fire**



**10 m LNG pool fire test on water performed at SNL, 2.5 m/s wind**



# Experiments

**Validation is difficult**

- **Few experiments have been designed specifically to study spreading**
  - **Typically laboratory scale**
  - **None have investigated wind, waves, currents, RPTs, height of release**
- **Data sets to date suggest a mass flux range for un-ignited pools of:**  
**0.029 – 0.195 kg/m<sup>2</sup>s (uncertainty not reported)**
- **Area in need of further research**



# Application of Models

**With the lack of experimental data on factors what can be done?**

- **Use appropriate models**
- **Perform verification and validation with available data**
- **Base safety margin on V&V outcome**



# Model Assessment

**First question to ask:**

**Does the model have sufficient physics?**

**Some examples:**

- **For confined pools a model should have physics to capture the effect of ice formation**
- **For spills that can be affected by surrounding objects a model should be able to have physics to capture irregularly shaped pools**

**Types of models available (see ref [1]):**

- **simplified integral balance (several variations)**
- **shallow-layer models**
- **computational fluid dynamic (CFD) codes**

[1] Luketa-Hanlin, A. (2006) A review of large-scale LNG spills: experiments and modeling, J. Hazardous Materials, A132, 199-140.



# Verification and Validation

**Verification:** Purpose is to check if equations are being solved correctly and if any errors exist.

**Validation:** Purpose is to determine if models contain appropriate and sufficient physics to predict the metrics of interest for a particular application.

- Part of the validation process is uncertainty quantification and sensitivity analysis
- Comprehensive documentation of V&V also important, describing model, experimental data, and steps taken to carry out process.



# Uncertainty Quantification

- Includes uncertainty arising from experimental measurement, as well as from model parameters
- The result will provide an estimate plus uncertainty for the metrics of interest
- Perform for comparison to data sets and extrapolated predictions
- Quantification can be performed using a sampling method such as Latin Hypercube available in the open source code, Dakota



# Sensitivity Analysis

- **Provides understanding of model behavior and identifies parameters which contribute to the largest uncertainty in response quantities**
- **This allows identification of areas where improvements to the model and/or experimental measurement can be made to reduce uncertainty**
- **Linear regression analysis is one method to assess sensitivity along with scatter plots**





# Final Step

**Must decide if model is adequate for intended use and what safety margin to apply**

- **If model is not adequate it may be necessary to
  - improve the model
  - use a different model and/or
  - obtain additional experimental data to reduce input uncertainties to the model**
- **Given the upper bound of the uncertainty range provided, a regulator will have to decide what margin of safety to apply based on the model, location, and reported range.**



# Recommendations

- **Use appropriate models for pertinent physical mechanisms.**
- **Apply V&V process: includes uncertainty quantification, sensitivity analysis, and documentation**
- **Base safety margin on V&V outcome**



# Pool Fire Description

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# Issues and Challenges

- Fires Are Low Momentum Phenomena
  - Easily disturbed by winds, objects, etc.
- Thermal Radiation Couples Vast Length Scales
  - Smoke shielding is likely related to flame structure

# Effect of Wind on Fires



9 m  
SNL

- Even light winds, 1-2 mph, create downstream vortical structures
- The structures do not form smoke as easily as ring structures
- The vortical structures are a result of ground/plume vorticity interactions, even isothermal jets form them – thus expect them for LNG fires.



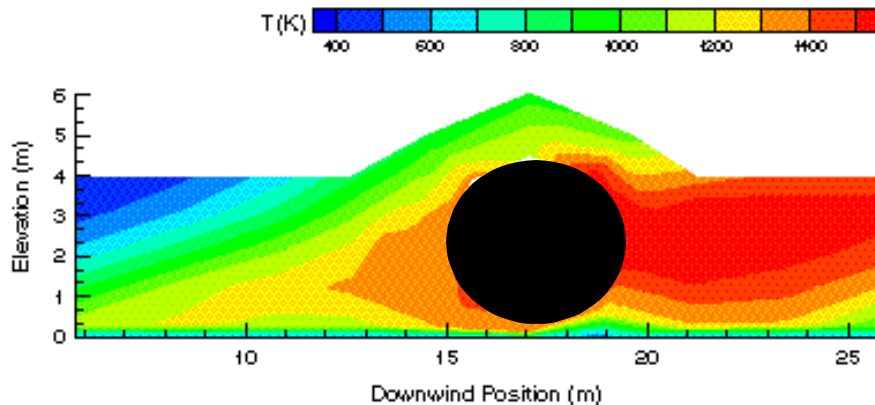
20 m  
SNL/  
NAWC



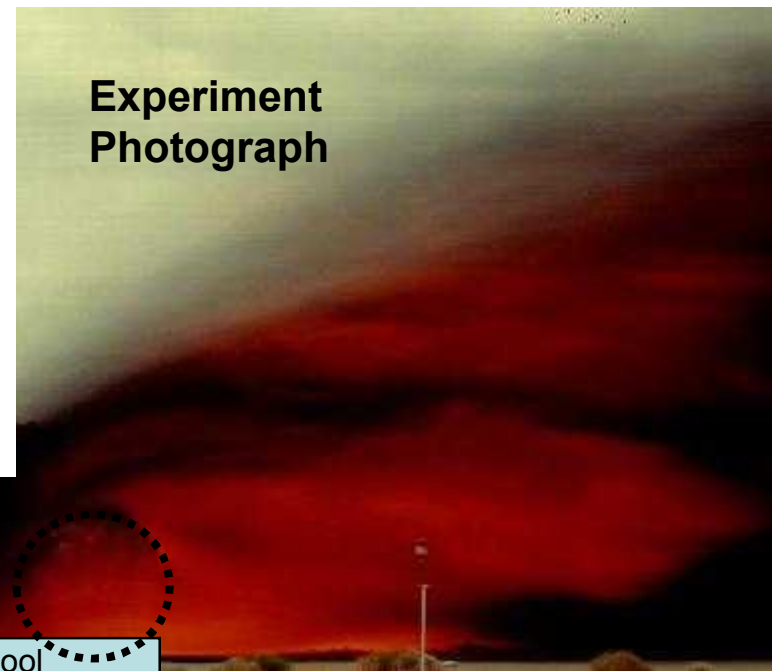
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# Objects Affect Fires

In general, fire/object interactions can result in significantly altered mixing rates and heat flux levels



**Experimental Data**



Fluxes up to  $450 \text{ kW/m}^2$  were measured in wake region of 4 m cylinder in 20 m diameter JP8 fire

- Factor of 3 greater than standard values



# Issues and Challenges

- Fires Are Low Momentum Phenomena
  - Easily disturbed by winds, objects, etc.
- Thermal Radiation Couples Vast Length Scales
  - Smoke shielding is likely related to flame structure



# Smoke Shielding – JP8 Examples

30 cm - SNL



2 m - SNL



3 m - SNL



5 m - SNL



10 m - SNL



20 m – SNL/NAWC

- Fires less than ~ 2m have no smoke shielding
- Smoke shielding increases with diameter



# Smoke Shielding – Methane/LNG

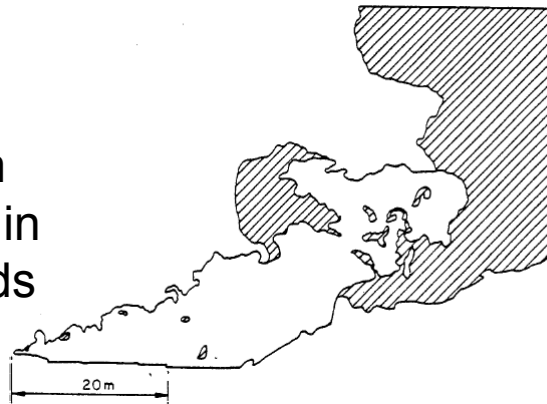
1 m  
SNL



10 m  
SNL



20 m  
Maplin  
Sands



35 m  
Montoir



- Trends are similar to JP8, but scales are ~10x larger
  - Below ~ 20 m, no smoke shielding
  - Smoke shielding appears to increase with increasing diameter



# Smoke Shielding

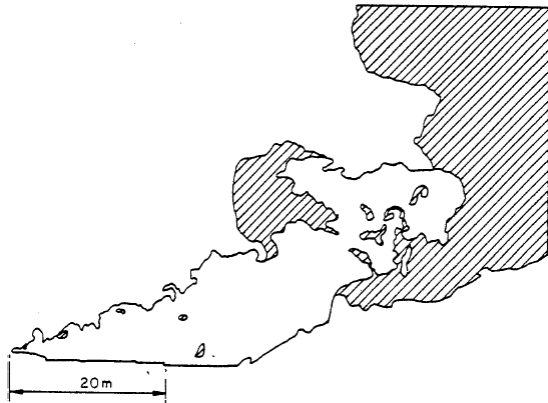
JP8 – 2 m



JP8 – 3 m



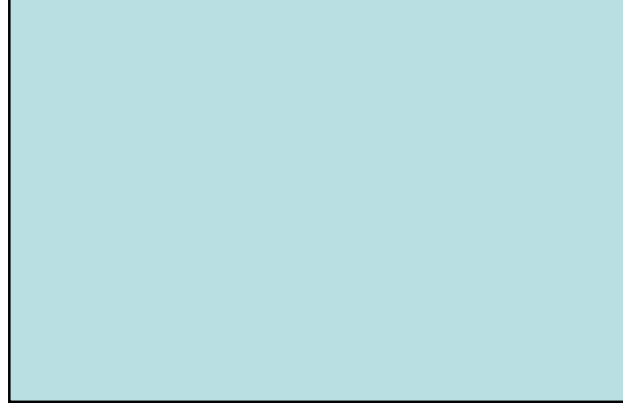
JP8 – 20 m



LNG – 20 m



LNG – 35 m



LNG ~ 200 m ?????

- The smoke shielding is expected to increase for large LNG fires



# What causes smoke shielding?

- Smoke shielding is likely due to quenching
  - ~ 1/3 to 1/2 energy loss in flames result in quench
  - Energy loss is an accumulation of radiation losses due to soot emission

$$s \bullet \nabla I(s) + \alpha I(s) = \frac{\alpha \sigma T^4}{\pi}$$

$$\alpha = f(kX_{soot}TL)$$

where

$k$  = Plank - Mean Specific Extinction Coefficient

$X_{soot}$  = Soot Volume Fraction

$T$  = Soot Temperature

$L$  = Path Length

- Source term for soot emission is heavily weighted to high-temperature regions of the fire, e.g. the flame sheets
- Two important parameters
  - Soot concentration
  - Soot temperature (most important)



# Soot Concentration

- Affects when the fire becomes optically thick
- Soot concentration is not constant in a fire
- Laminar Flame Data (Peak Concentration)
  - Methane 0.2 ppm
  - Propane 2 ppm
  - Ethylene 8 ppm
- Radiation is linear in soot concentration for optically thin fires. Methane has an order of magnitude less soot than higher hydrocarbons and appears to need an order of magnitude larger fire to become optically thick.

$$s \bullet \nabla I(s) + \alpha I(s) = \frac{\alpha \sigma T^4}{\pi}$$

$$\alpha = f(kX_{soot}TL)$$

where

$k$  = Plank - Mean Specific Extinction Coefficient

$X_{soot}$  = Soot Volume Fraction

$T$  = Soot Temperature

$L$  = Path Length

# Flame Sheet Structure ~ 2 mm thick

10-  
100 nm  
Soot



Agglomeration

Surface Growth &  
Coagulation

**Thermophoretic  
Forces**

Condensate  
(nm dia.)  $C_{100}$ 's

PAH Rings  $C_{10}$ 's

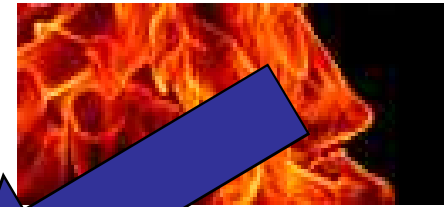
Fuel  
 $C_{12}$

$C_2$ - $C_3$

$CO_2$   
 $H_2O$

$CO_2$   
 $H_2O$

Air



Soot Emission Zone

Primary Heat Release Zone

**Differential  
Diffusion**

Soot is formed in  
a ~ 1000 K/mm  
temperature  
gradient. A mean  
1/4 mm shift = a  
factor of 2 in  
radiation !!!!



# Technical Basis for LNG Predictions

- **Application requires an extrapolation in scale**
  - **An order of magnitude extrapolation**
  - **Complex physics environment where fundamental mechanisms are not proven**
  - **Public safety is involved**
- **Low momentum phenomena**
  - **Flame shape changes with environment**





# Recommendations

- **Best practice**
  - Take data at larger scale
- **Required practice**
  - Uncertainties must be carried with prediction, particularly in the absence of data
    - In a performance-based regulatory environment, expect uncertainties to be evaluated along with predictions
    - Anay will address this point in detail in her talk
- **Suggested practice**
  - Use CFD for noncircular pool fires



# Pool Fire Modeling: Radiation

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June 13, 2007

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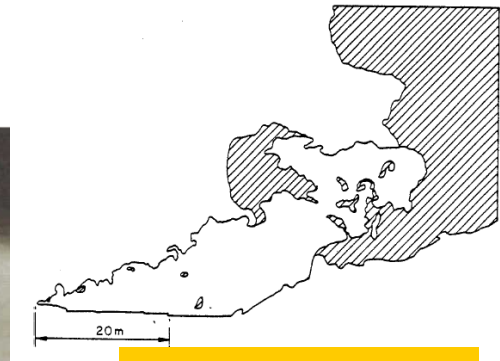


# LNG Smoke Production

- LNG fires do not smoke like typical hydrocarbons at scales tested to date (35 m diameter or less).
- Some smoke production evident in largest LNG fires at vertical locations high above the ground.
- We expect smoke shielding to occur in LNG spill fires of very large diameter (100's of meters), but no data at these scales.
- Emissive power data inconclusive -  $q'' \sim 170 - 270 \text{ kW/m}^2$  for LNG;  $q'' \sim 20 - 40 \text{ kW/m}^2$  for other fuels.
- Radiative fraction data inconclusive - 0.16 versus 0.36 for essentially identical LNG pools.



Montoir 35 m  
LNG pool fire



Maplin Sands  
20 m LNG pool  
fire

SNL – 7.9 m  
JP-8 pool fire

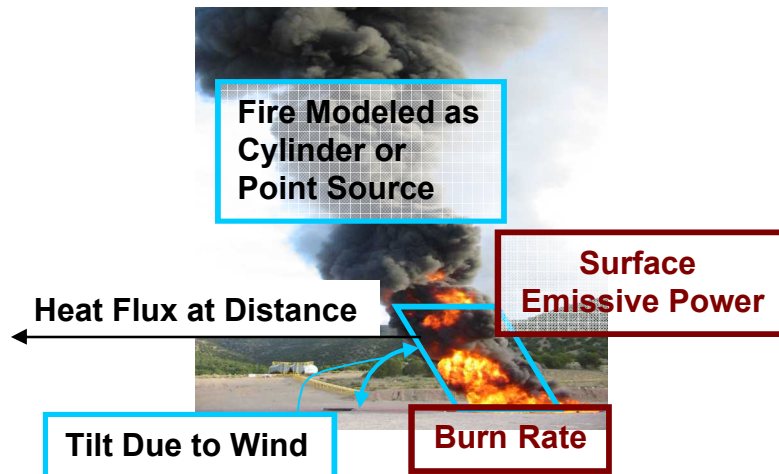


SNL – 10 m  
LNG pool fire

# LNG Pool Fire Modeling

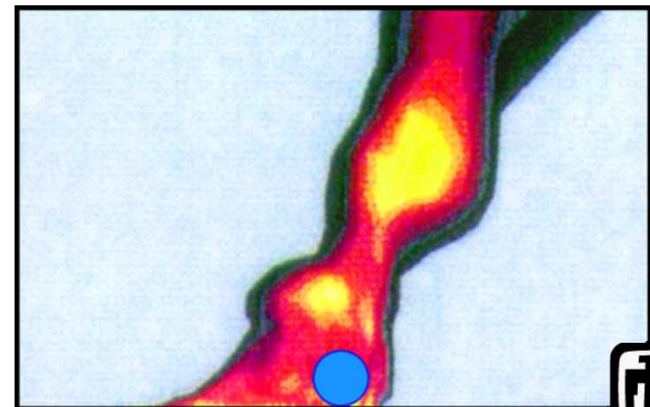
## Integral or Similarity Models

- Treats fire as a global emitter with typically assumed cylindrical shape
- Input parameters based on data
- Heat flux ( $\text{kW/m}^2$ ) calculated at distance
- Good for long distances, simple geometries



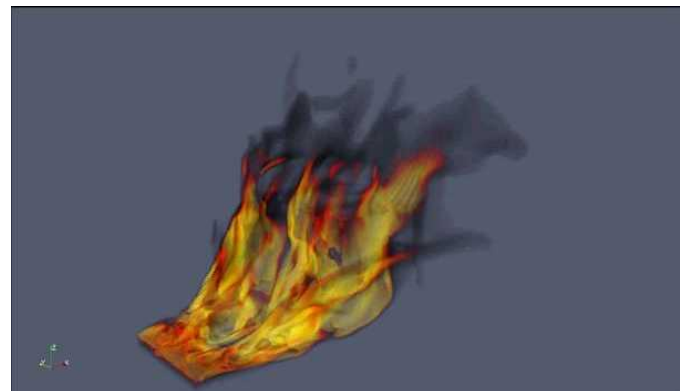
## Computational Fluid Dynamics (CFD) Models

- Invokes more first principles
- Flow, reactions, heat transfer modeled
- Calculates heat flux distributions for specified scenario including complex geometries and irregular shaped pools



# Fire modeling considerations

- Validation needed for smoke shielding, flame height/diameter ratio, and burn rate for any model.
- Reasonable approach using solid flame models for locations far from populations.
- In areas where thermal interactions occur with structures - CFD models are necessary.
  - Assess building shielding on short-term hazards.
  - Assess latent effects of fire on structures and people and emergency management needs.



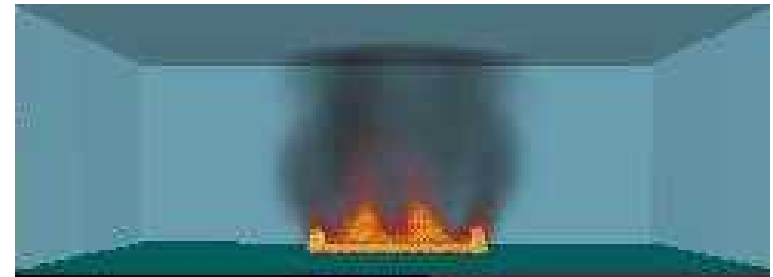
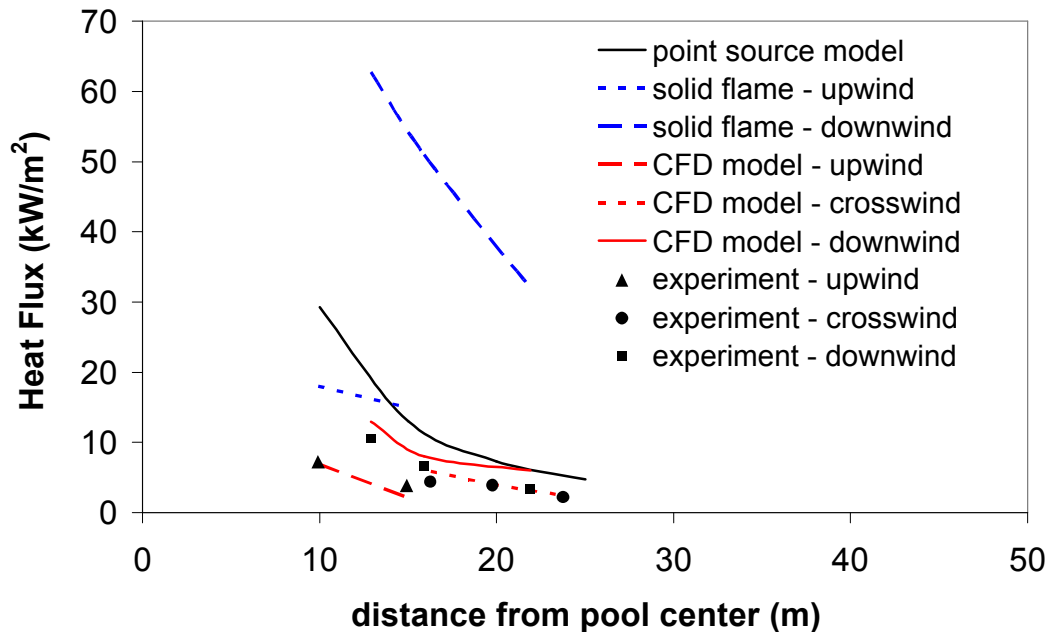
CFD simulation of object/fire interaction using FUEGO (cross-wind facility)



CFD simulation using FUEGO of 3 m JP-8 pool fire in Thermal Test Complex

# Non-circular pools

A trench fire is a pool fire with an elongated rectangular configuration. Croce, et. al. performed thirteen tests with trench sizes ranging from 0.98 x 4.4 m to 3.9 x 52.1 m using LNG.



**15.52 x 1.82 m trench fire.**  
**Solid flame models assume**  
**circular fire. Vulcan, Sandia**  
**CFD fire code, used for**  
**simulation**



# **LNG pool fire data for validation at relatively small scale**

## **Trench Fires up to 52 m:**

Croce, P.A, Mudan, K. S., and Moorhouse, J. (1984) Thermal Radiation from LNG Trench Fires – Vol 1 and 2, Arthur D. Little, Inc., GRI Report No. 84/0151.1

## **Circular Pool Fires up to 35 m in diameter:**

- Nedelka, D. et al., (1989) The Montoir 35 m diameter LNG pool fire experiments, Int. Conf. Liq. Nat. Gas, v. 2, 9th, 17-20 Oct 1989, Nice, France.

- Mizner, G. A., Eyre, J. A. (1982) Large-Scale LNG and LPG Pool Fires, EFCE Publication Series (European Federation of Chemical Engineering), no.25, p.147-163.

## **Pool Fire on Water up to 15 m in diameter:**

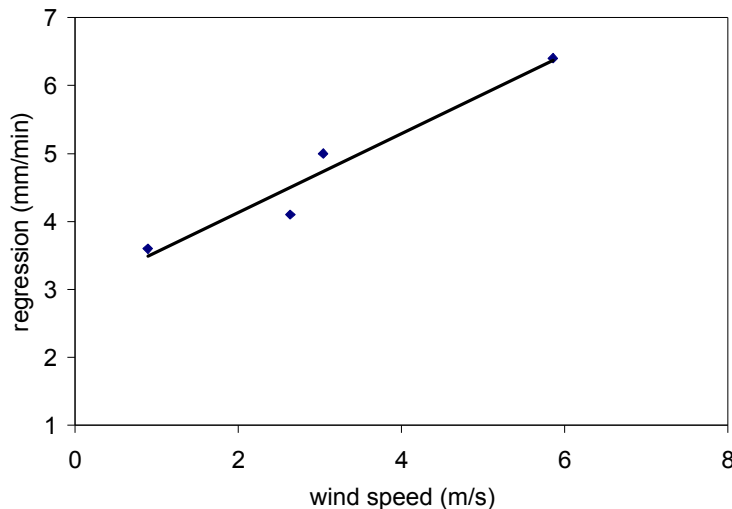
Raj, P. K., Mudan, K. S., Moussa, A. N. (1979) Experiments Involving Pool and Vapor Fires from Spills of LNG on Water. Report #CG-D-55-79, NTIS AD077073, U.S. Coast Guard.

# Parameters for solid flame models

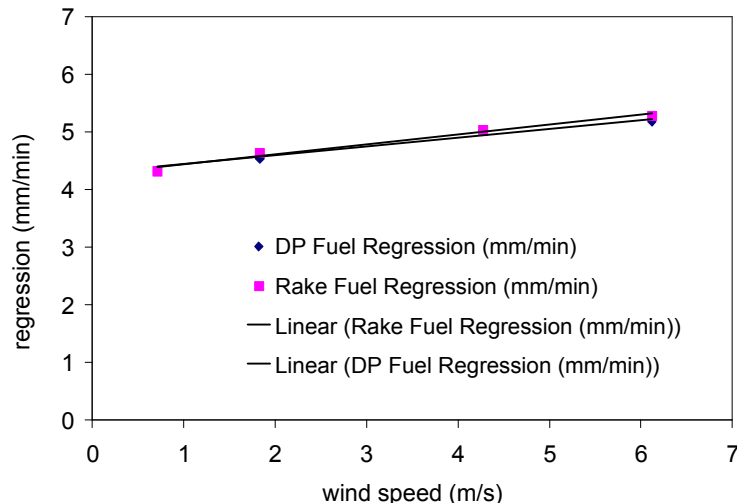
**Burn rate:** Data indicates,

- $2.6 \times 10^{-4} - 9 \times 10^{-4}$  m/s (fire tests on water)
- $3.4 \times 10^{-4} - 7.1 \times 10^{-4}$  m/s (additive from fire tests on land and un-ignited pools)
- Recommend using a range of  $3 \times 10^{-4} - 8 \times 10^{-4}$  m/s

**Variability could be due to the effect of wind:**



18.9 m, JP-8 pool fire



7.9 m, JP-8 pool fire



# Parameters for solid flame models

## Flame Height: Data and correlations

Diameter (m)	Experiment (L/D) <sub>AVERAGE</sub>	L/D predicted					
		Pritchard	Moorhouse	Thomas	Zukoski*	Steward*	Heskestad*
<b>8.5</b> (test 1 china lake)	<b>2.8</b>	<b>2.8</b>	<b>2.0</b>	<b>3.0</b>	<b>4.7</b>	<b>4.1</b>	<b>3.6</b>
<b>9</b> (test 4 china lake) (2.2 m/s)	<b>2.8</b>	<b>2.6</b>	<b>1.9</b>	<b>2.5</b>	<b>3.9</b>	<b>3.7</b>	<b>3.1</b>
<b>20</b> (Maplin Sands - land) (6.2 m/s)	<b>2.15</b>	<b>2.2</b>	<b>1.6</b>	<b>1.6</b>	<b>2.9</b>	<b>3.1</b>	<b>2.4</b>
<b>35</b> (Montoir) (9 m/s)	<b>2.2</b>	<b>2.2</b>	<b>1.6</b>	<b>1.5</b>	<b>2.9</b>	<b>3.1</b>	<b>2.4</b>

$$\frac{L}{D} = a \left[ \frac{\dot{m}''}{\rho_a \sqrt{gD}} \right]^b$$

**Dimensional Analysis form used by Thomas, Moorhouse, and Pritchard.**

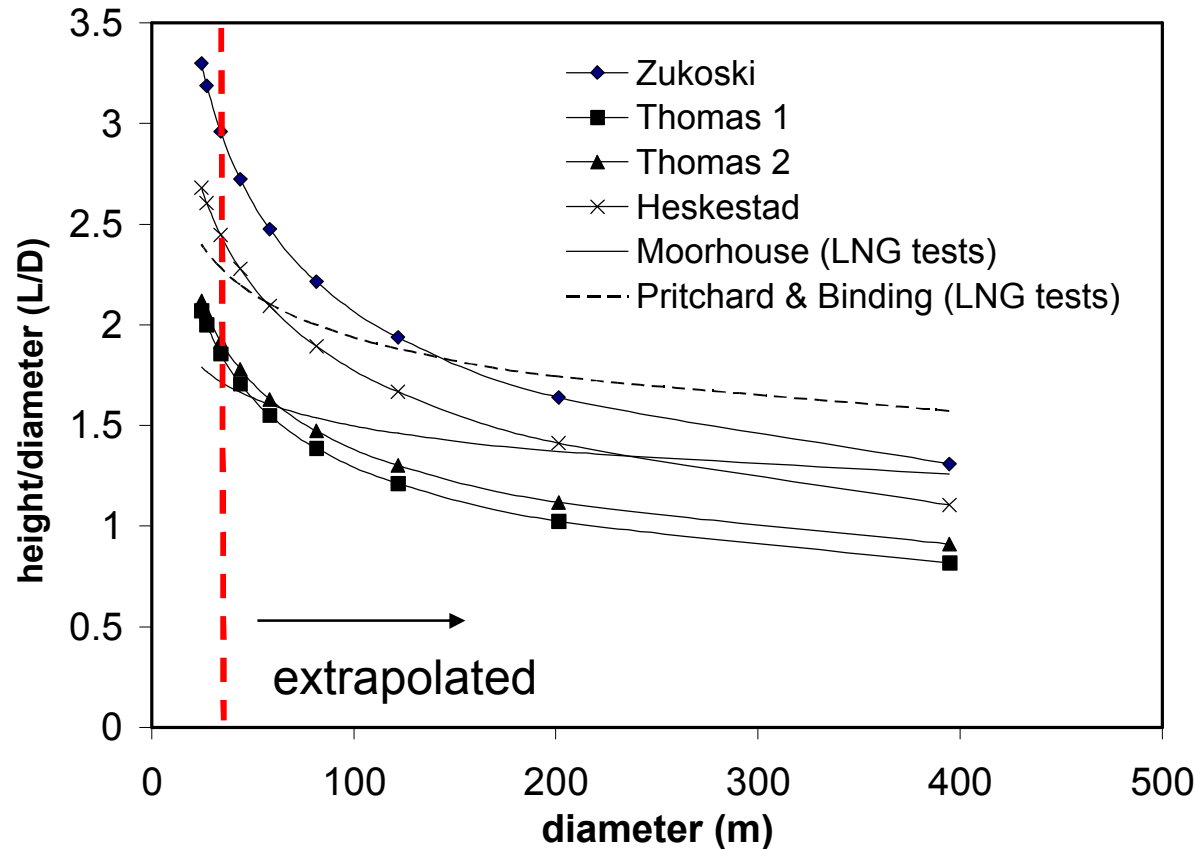
**Determined constants a and b from:**

- Thomas: 2 m wood crib fires
- Moorhouse: 6.9 – 15.4 m LNG pool fire land tests
- Pritchard and Binding: LNG and other hydrocarbon pool fires from 6.1 – 35 m

# Parameters for solid flame models

## Flame Height Correlations

- Extrapolated flame height/diameter ratio ( $L/D$ ) is between 1 – 2.
- Realize the large extrapolation.
- Also, realize that “flame height” defined within the context and range of these correlations may be meaningless for pools on the order of 100 m.
- Recommend using a range of 1 – 2 for  $L/D$





# Parameters for solid flame models

**Surface Emissive Power:** Data indicates,

Study	Spill terrain	Pool Diameter (m)	SEP (kW/m <sup>2</sup> )
U.S.CG China Lake Tests	Water	15	210 ± 20 (narrow gauge) 220 ± 50 (wide gauge)*
Maplin Sands	Land	20	177 – 219 (narrow gauge) 140 - 180 (153 average)* (wide gauge)
Montoir	Land	35	290-320 (narrow gauge) 257-273 (wide gauge) (non-idealized flame) Idealized: 175 ± 30*

**\*Idealized flame calculations using the Thomas correlation. If the Moorhouse correlation was used, then a higher SEP would have been calculated for the LNG tests on water.**

# Parameters for solid flame models

## Surface Emissive Power:

Small-scale tests have indicated that the SEP decreases along the height of the flame due to the production of smoke. It is often approximated as a decreasing monotonic function with height.

*Is this always true?*

- Can depend on scale:

For 30 m and 50 m kerosene fires, Takahashi et al. [1], reported that the probability of the luminous zone was maximum at approximately 1 diameter from the pool surface then decreased

- Can depend on environment:

The effect of wind and topography can change the SEP profile with height

Indicates difficulty in predicting the magnitude and profile of SEP for large-scale LNG pool fires

[1] Takahashi, N., et al. (1999) Behavior of luminous zones appearing on plumes of large-scale pool fires of kerosene, Fire Safety J., 33, 1-10.



# Parameters for solid flame models

## Surface Emissive Power:

- Realize that the (SEP, flame height) combination applicable to LNG pool fires on the order of 100 m is unknown due to the large extrapolation and cannot be based on a single SEP value or particular correlation at small scale.
- It is suspected that the SEP would be below 200 kW/m<sup>2</sup>, but the extent is unknown. Could be 50, 100, 150 kW/m<sup>2</sup> or possibly higher if wind effects are taken into account.
- Since public safety is involved and due to the uncertainty, we recommend a conservative range of values.
- Until additional data is obtained to reduce uncertainty it is recommended that a conservative range of  $220 \pm 50$  kW/m<sup>2</sup> is used.



# Parameters for solid flame models

## Flame tilt and drag:

- Flame tilt and drag have been observed in both the Maplin Sands and Montoir LNG land tests, as well as the tests performed by Moorhouse. The China Lake tests on water reported flame tilt and the pool shape was elliptical.
- The correlations developed by A.G.A. and Moorhouse to predict flame tilt and drag for integral models have been developed from LNG pool fire land tests
- A variability of  $\pm 30\%$  of calculated values for flame tilt and drag should be included to account for the variability demonstrated from test data.

## Transmissivity:

- Consider a range of values from 0.5 to 0.9 as found from China Lake tests. Note that the transmissivity is a function of humidity and distance.
- A variability of  $\pm 30\%$  should be included in transmissivity functions to account for experimental uncertainty



# Recommendations

- **Use CFD model for locations where fire could interact with surrounding objects. Integral models acceptable for locations far from populations**
- **For solid flame models use a range of values**
- **Apply V&V process: includes uncertainty quantification, sensitivity analysis, and documentation**
- **Base safety margin on V&V outcome**