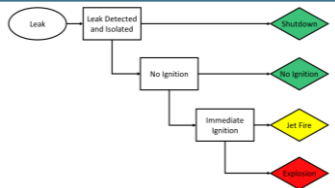
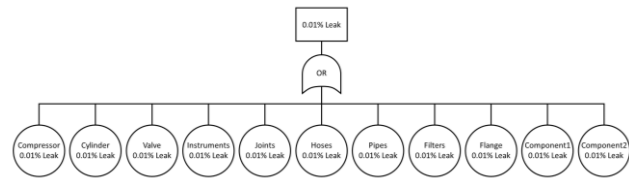
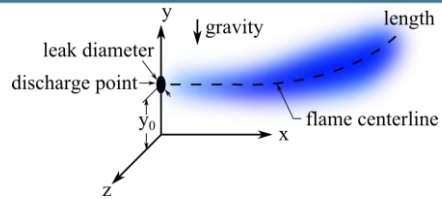




Hydrogen Plus Other Alternative Fuels Risk Assessment Models (HyRAM+) for LNG Facilities



Brian Ehrhart, Dusty Brooks, and Ethan Hecht

Project: PHMSA support for safety, regulation, production, distribution, and use of Liquefied Natural Gas (Contract 693JK320N0000030001)

Task 1: LNG Modeling - Final Task Presentation

March 3, 2022

Acknowledgements



For this work, the addition of cryogenic methane to HyRAM+ risk and physics models was done by:

- Brian Ehrhart, Ethan Hecht, Dusty Brooks, Garret Mulcahy, and Cianan Sims

HyRAM+ relied on input and model validation from:

- Cyrus Jordan, Jessica Shum, Scott Egbert, Xuefang Li, and Myra Blaylock

This presentation describes HyRAM+, a revised version of the HyRAM software, which itself was built upon the previous work of many others. Past contributors to HyRAM include:

- Katrina Groth, John Reynolds, Erin Carrier, Greg Walkup

The development of HyRAM+ was supported by:

- U.S. Department of Energy (DOE) Office of Energy Efficiency (EERE) Hydrogen and Fuel Cell Technologies Office (HFTO)
- DOE EERE Vehicles Technologies Office (VTO)
- U.S. Department of Transportation (DOT) Pipeline and Hazardous Materials Safety Administration (PHMSA)

Challenge Addressed and Project Objectives



Challenge Addressed:

- Safety regulatory requirements for the production, distribution, and use of liquefied natural gas (LNG) should be based on a sound technical basis, including validated software for risk and consequence modeling

Overall Project Objective:

- Sandia National Laboratories (Sandia) will engage in analytical studies, computational modeling, quantitative risk assessments, advanced technology assessments, and systems engineering research, development and demonstrations in support of the U.S. Department of Transportation (DOT) Pipeline and Hazardous Materials Safety Administration (PHMSA) objective to enhance the safety, regulation, production, distribution, and use of Liquefied Natural Gas (LNG).

Task Objective, Budget, and Scope



Task 1: LNG Modeling Objective:

- Sandia will provide reduced-order models that characterize natural gas releases from pressurized systems. This specifically includes characterizing the resulting jet plume from liquefied natural gas releases that may include gaseous, liquid, or mixed-phase flow. The characterization models will be capable of estimating unignited jet plume extent and concentration, as well as ignited jet flame heat flux and temperature. The models will be available as open source code, as well as within a graphical user interface that can run quickly on standard computing resources.

Task 1 Deliverable:

- Sandia will provide open source reduced-order LNG Models with graphical user interface, downloadable from Sandia GitHub
- Sandia will provide documentation on model operations and assumptions, including algorithm and user guide

Task Funding: \$129k

Approach



Modify existing software: Hydrogen Risk Assessment Models (HyRAM)

- These reduced-order engineering models were originally based on gaseous hydrogen
- Efforts through other projects were adding ability to model liquid hydrogen (DOE HFTO) and CNG/propane (DOE VTO)
- This project would focus on adding ability to assess LNG risk and model LNG consequences

Modify consequence models:

- Modify source code to utilize cryogenic methane as a proxy for LNG
- Validate modified source code models with experimental data in literature

Modify risk models:

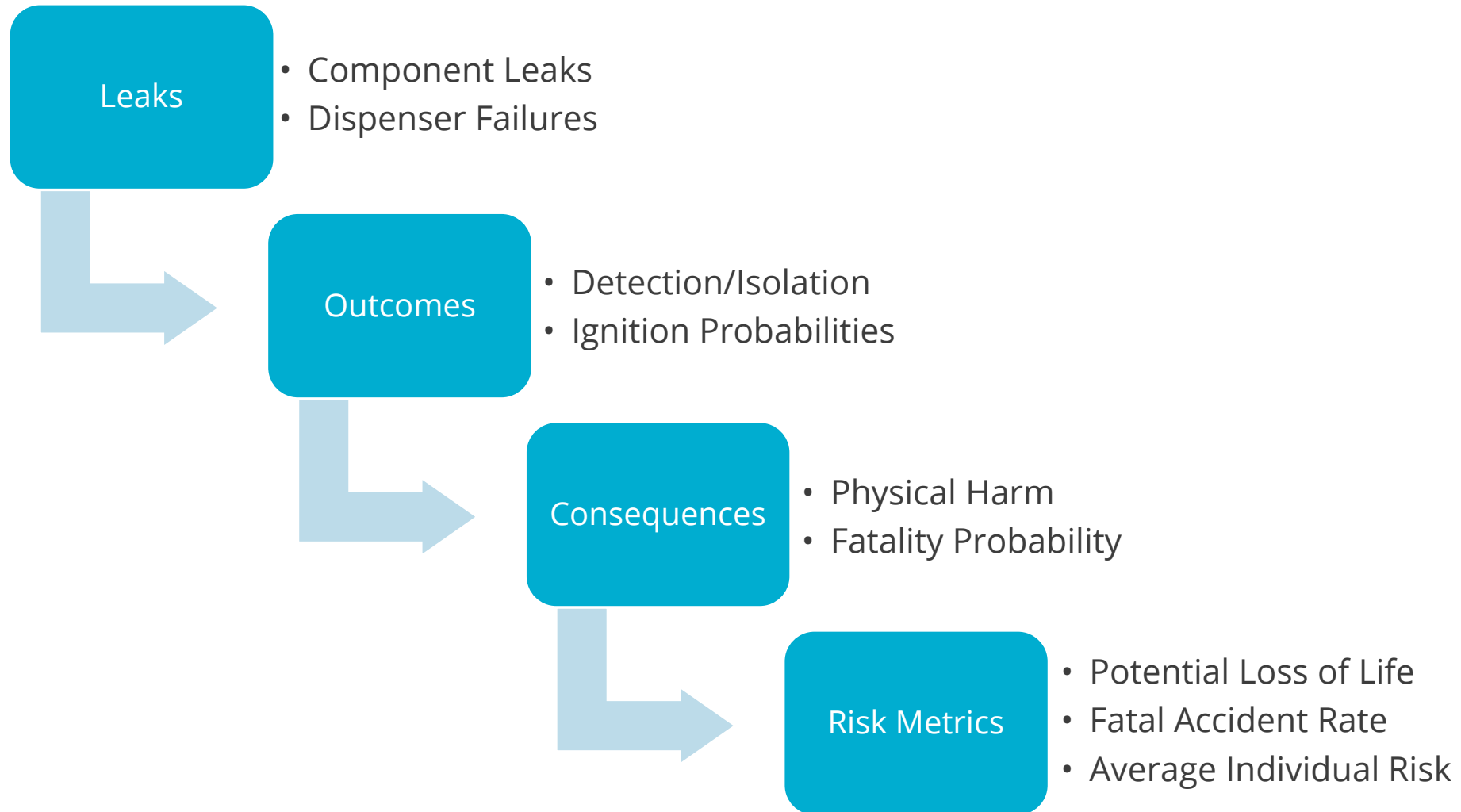
- Modify leak frequencies based on LNG-specific data
- Risk assessment also utilizes consequence models



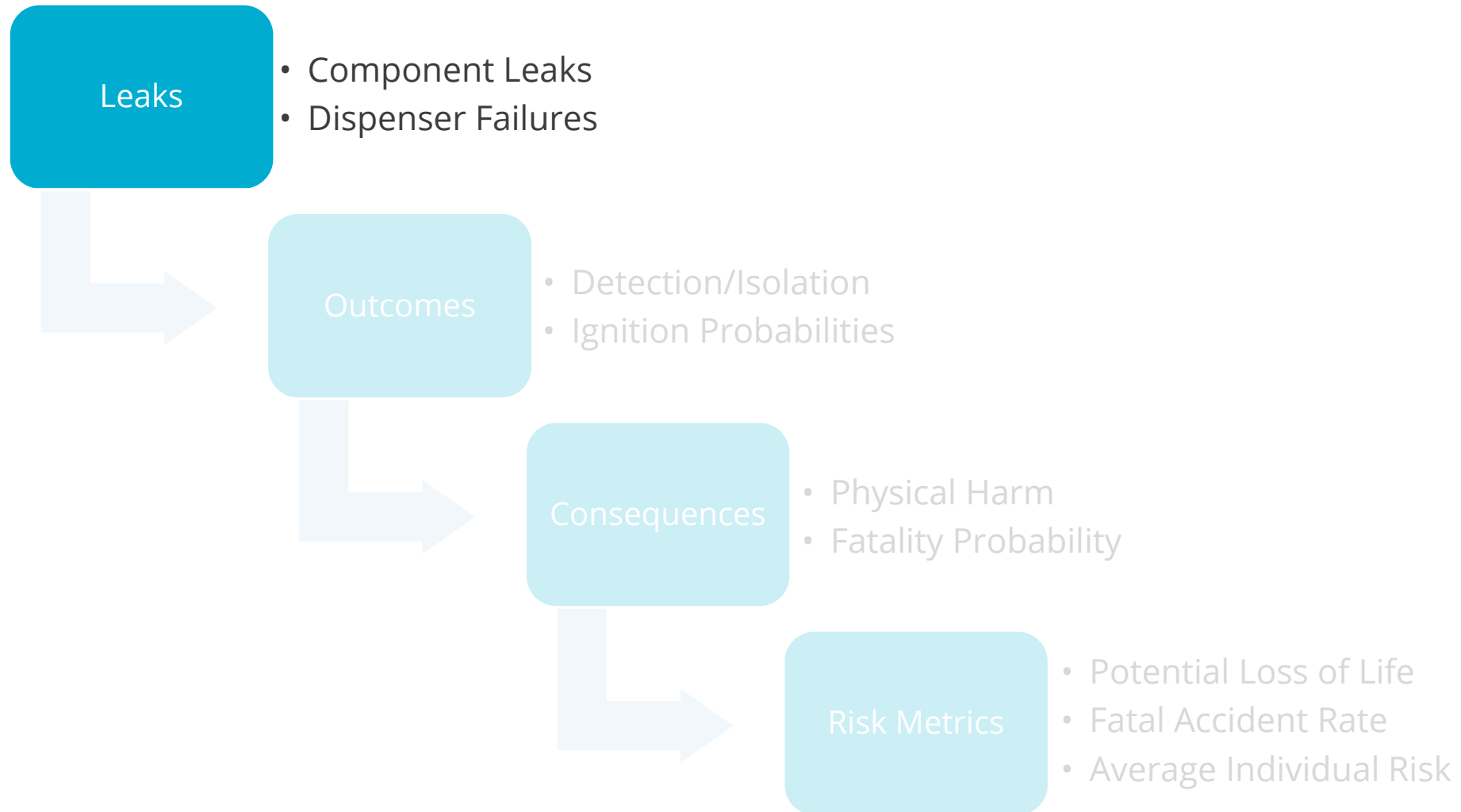
Overview of HyRAM+ Risk Assessment and Consequence Models



Overview of Risk Calculations in HyRAM+



Overview of Risk Calculations in HyRAM+



Leak Frequencies – Fault Tree



Random Releases

- Frequency of leaks of size k for i different components:
- $f_{random,k} = \sum_i N_{component} f_{leak,ik}$

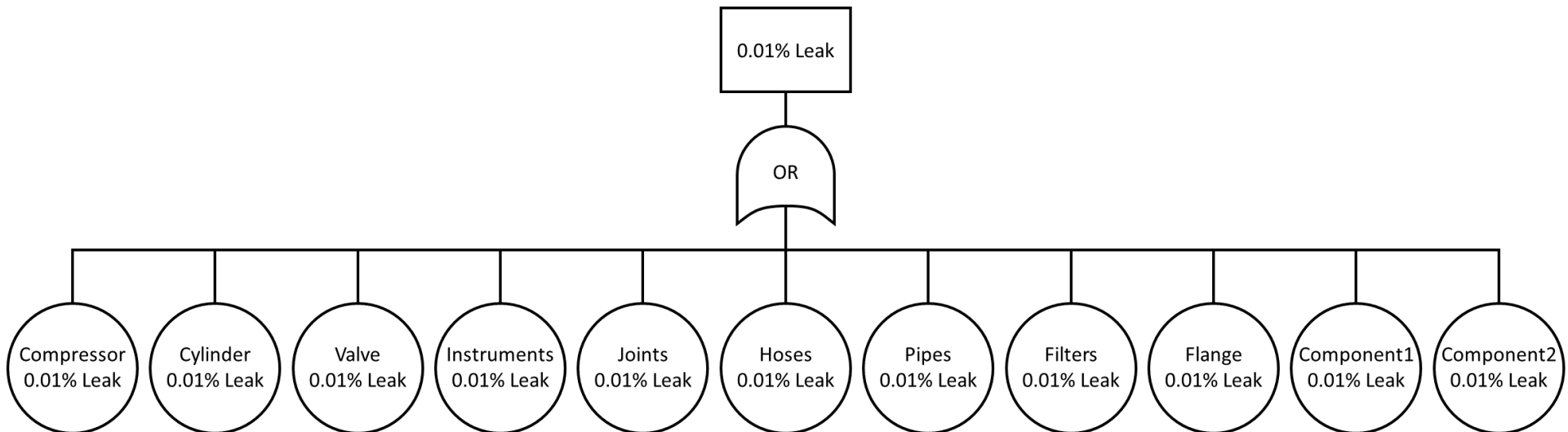
5 leak sizes, 9+ component types

- 0.01%, 0.1%, 1%, 10% 100% of pipe flow area

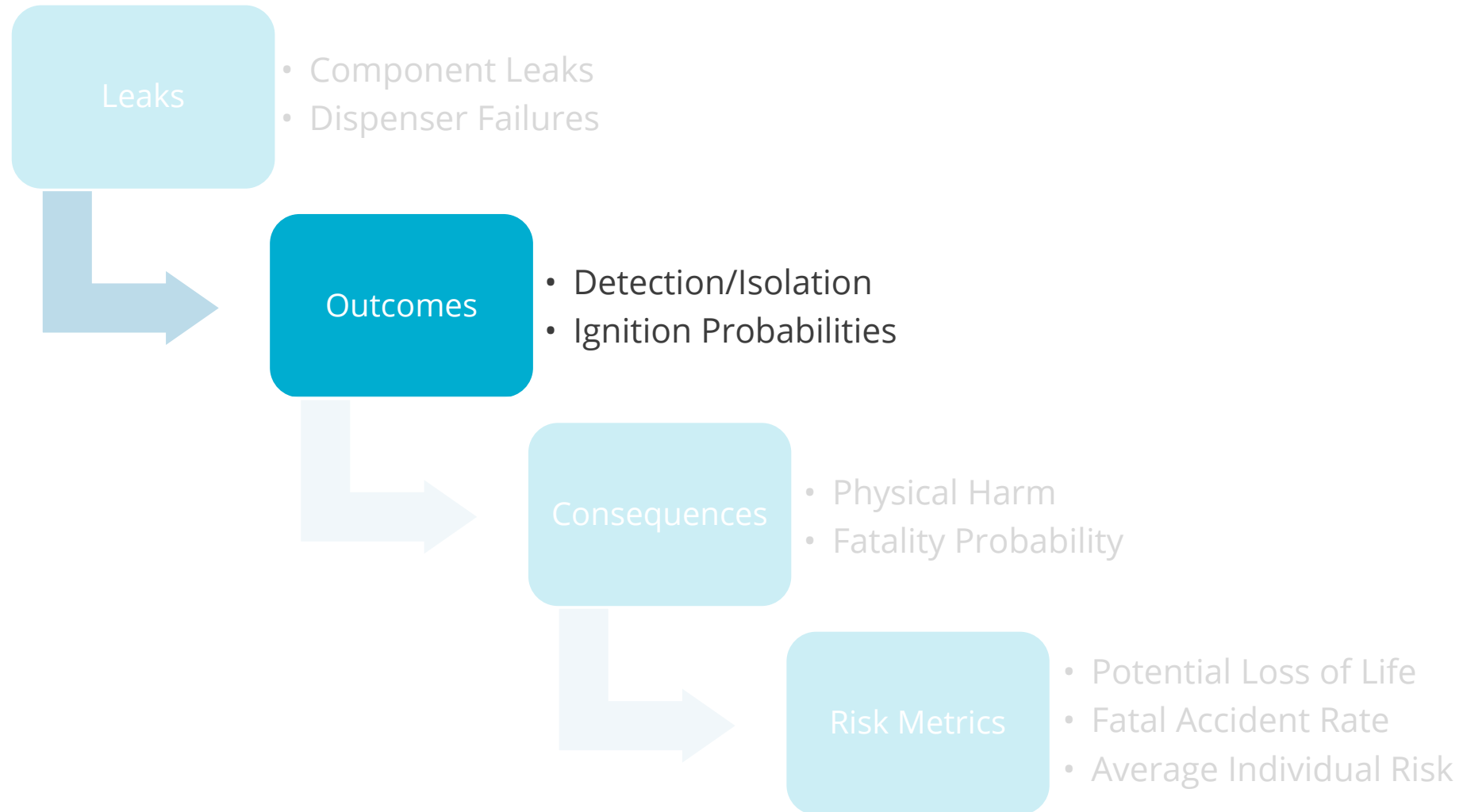
Dispenser Failures (100% leak size only)

- (slightly) more complicated fault tree

Overall leak frequencies can also be input directly



Overview of Risk Calculations in HyRAM+



Leak Outcomes – Event Tree

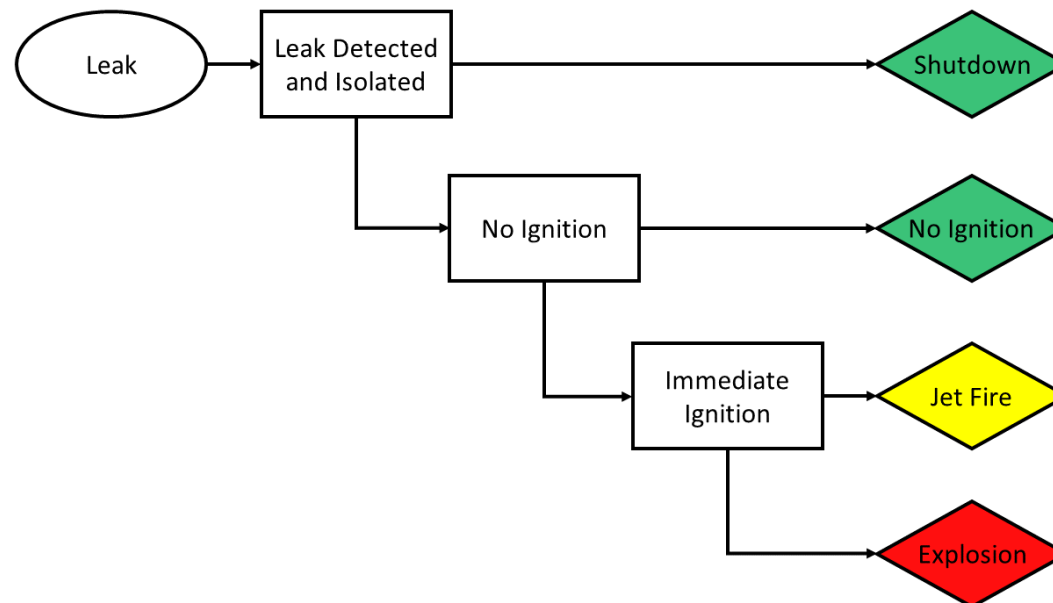


Probabilities on what could happen given a leak

- 4 outcomes possible

Leak detection and isolation credit is single input (0.9 default)

Immediate and delayed ignition probabilities as a function of flow rate (calculated)



Ignition Probabilities



Based on historical ignition probability data for methane (Cox, Lees, & Ang)

Modified for hydrogen:

- Reduce leak flow ranges by a factor 8
 - Allowing for differential molecular weight CH₄ vs H₂, which directly affects the size of flammable cloud
- Increase ignition probabilities by 16%
 - Allowing for the ratio of the flammable range of H₂ vs CH₄
 - Allowing that 15-75 vol% constitutes only 16% of total cloud size above lower flammability limit (from modeling)
- Assume immediate to delayed ignition probabilities are 2:1
 - Total ignition probability is immediate and delayed probabilities added together

HyRAM+ software GUI will notify users that default H₂ ignition probabilities should be modified when “methane” is selected as fuel type

Original Hydrocarbon Ignition Probabilities

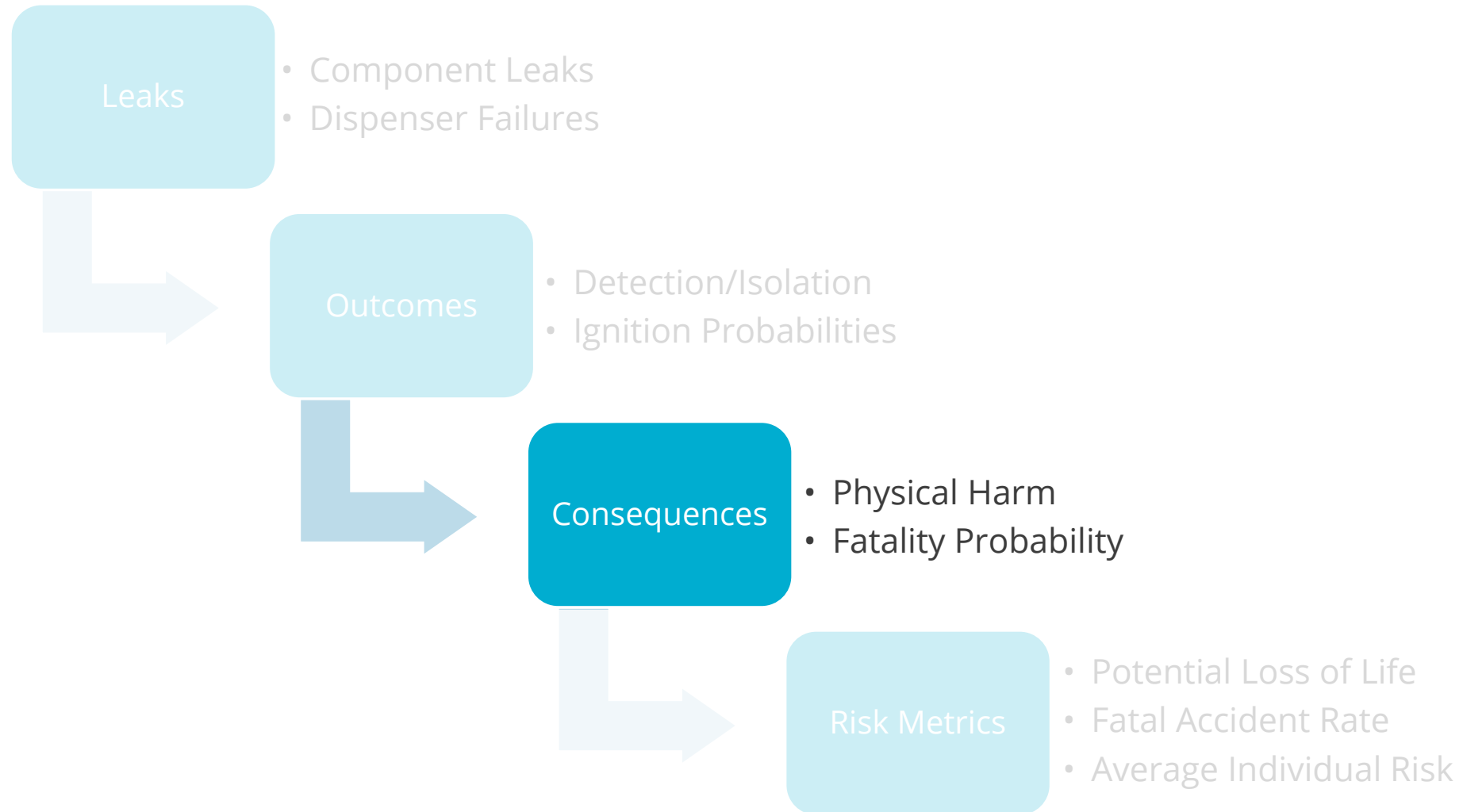
RELEASE RATE CATEGORY	RELEASE RATE (kg/s)	GAS LEAK	CRUDE	CLASS I	CLASS II	CLASS III
Small	< 1	0.010	0.010	0.006	0.004	0.002
Large	1 - 50	0.070	0.030	0.018	0.012	0.007
Massive	> 50	0.300	0.080	0.049	0.031	0.018

Estimated Hydrogen Ignition Probabilities

H ₂ Release Rate (kg/s)	<i>P</i> (Immediate Ignition)	<i>P</i> (Delayed Ignition)
<0.125	0.008	0.004
0.125 - 6.25	0.053	0.027
>6.25	0.230	0.120

A. V. Tchouvelev, “Knowledge gaps in hydrogen safety: A white paper,” International Energy Agency Hydrogen Implementing Agreement Task 19, Tech. Rep., January 2008.

Overview of Risk Calculations in HyRAM+



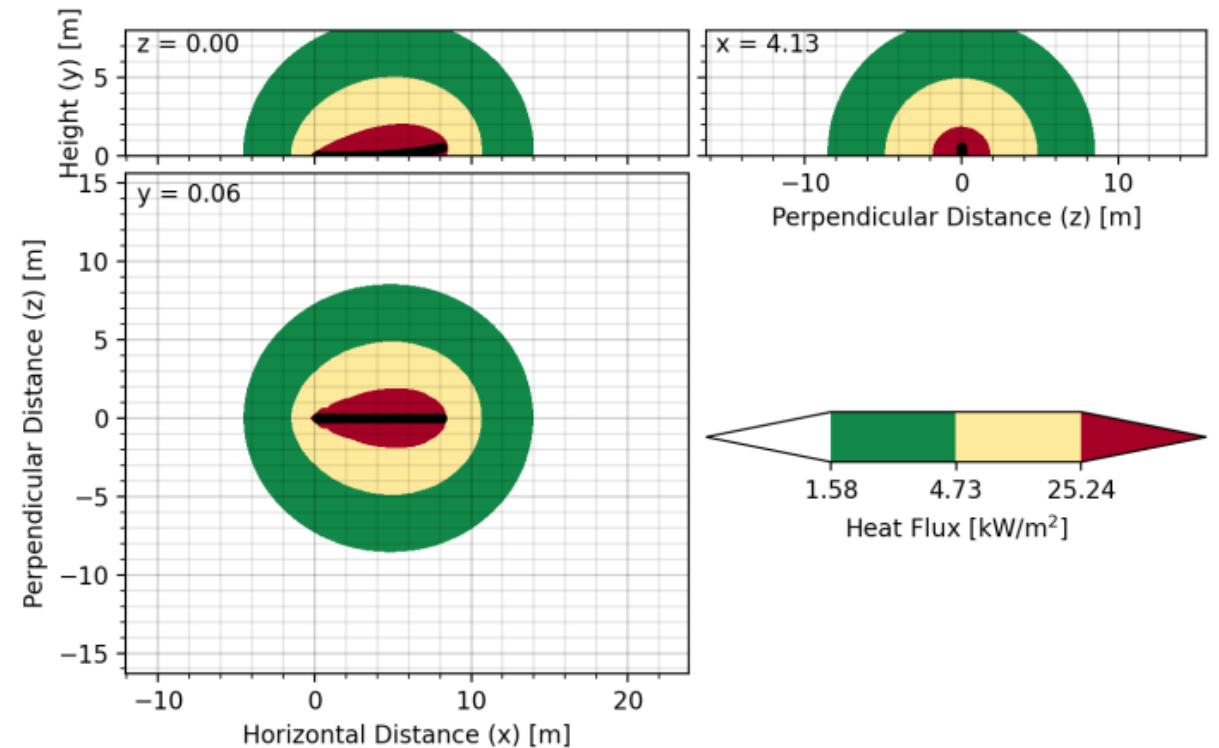
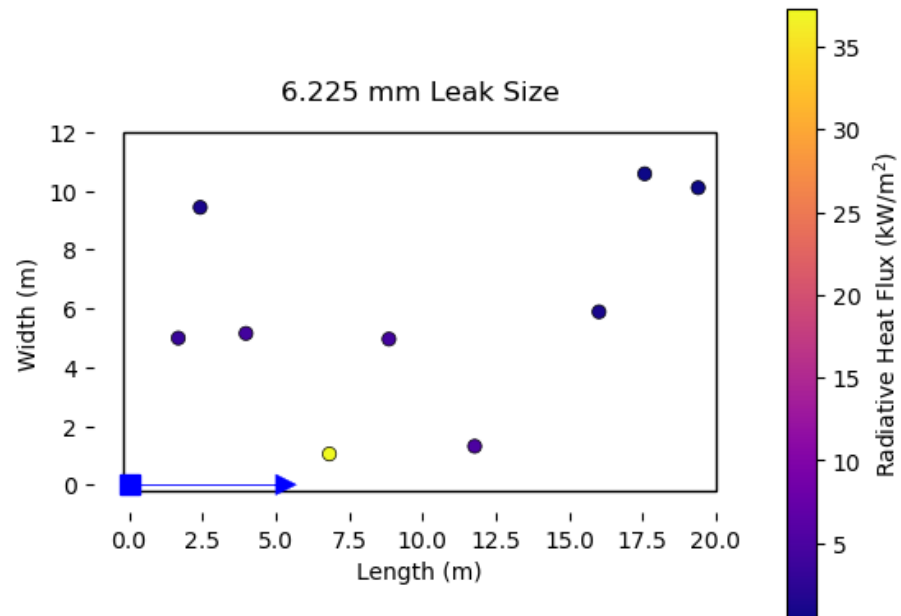
Thermal Harm from Jet Fire Heat Flux



Based on Jet Flame Physics model

Determines heat flux from leak at every occupant point

- For each leak size



Overpressure Harm – Basic Inputs



Peak overpressure and impulse are specified for each leak size

- User must determine values themselves or use defaults

These values are applied to each occupant position

- Regardless of distance away from leak

Units: Pa

	Variable	0.01% Leak	0.1% Leak	1.0% Leak	10% Leak	100% Leak
▶	Peak Overpres...	2500.0000	2500.0000	5000.0000	16000.0000	30000.0000
	Impulse	0.0000	0.0000	0.0000	0.0000	0.0000

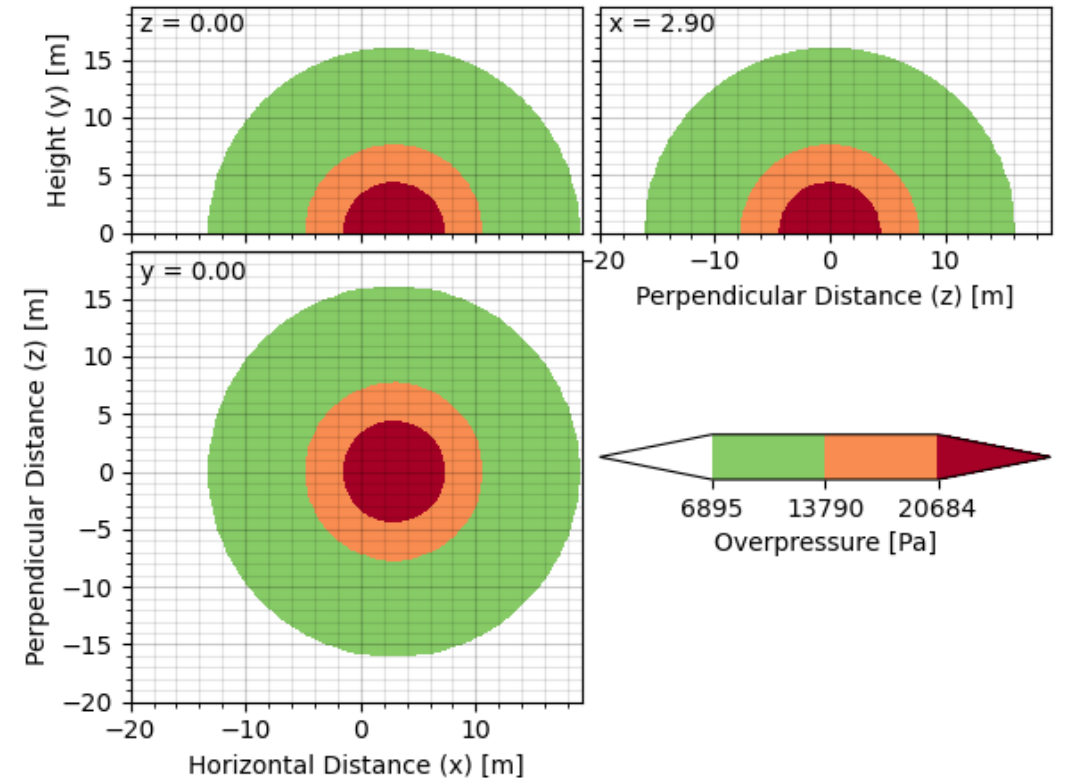
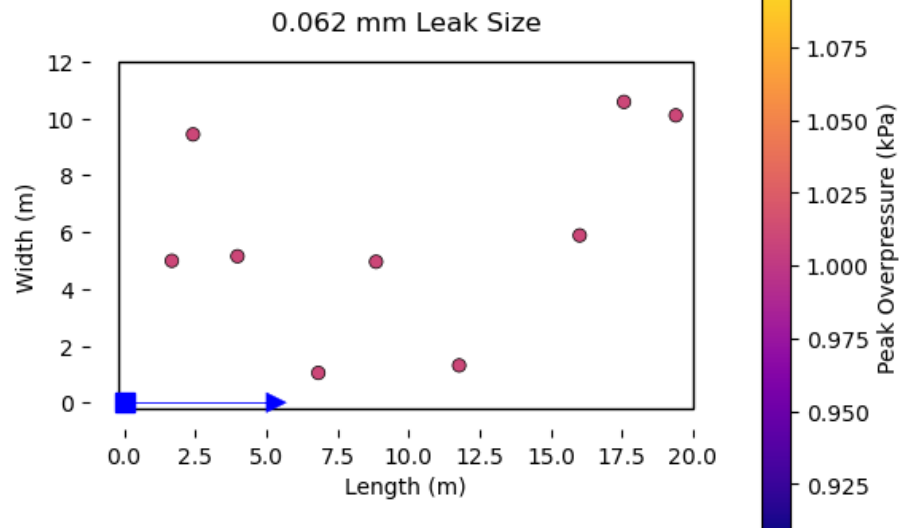
*Models to calculate overpressure and impulse
to be incorporated into risk calculations soon!*

Overpressure Harm – Unconfined Overpressure



- Based on Unconfined Overpressure model
 - Uses information from unignited jet plume
- Multiple overpressure models to choose

Coming in HyRAM v4.1



Thermal Fatalities – Thermal Probit Models



For each occupant,

Calculation of probability of a fatality ($P(\textit{fatality})$) based on probit value (Y):

- $P(\textit{fatality}) = \textit{Normal CDF}(Y|\mu = 5, \sigma = 1)$

Calculated from Thermal Dose Unit (V) based on heat flux (I) and exposure time (t):

- $V = I^{4/3}t$

Model	Equation
Eisenberg *	$Y = -38.48 + 2.56\ln(V)$
Tsao & Perry	$Y = -36.38 + 2.56\ln(V)$
TNO	$Y = -37.23 + 2.56\ln(V)$
Lees	$Y = -29.02 + 1.99\ln(0.5V)$

* default

Overpressure Fatalities – Overpressure Probit Models



For each occupant,

Calculation of probability of a fatality ($P(\text{fatality})$) based on probit value (Y):

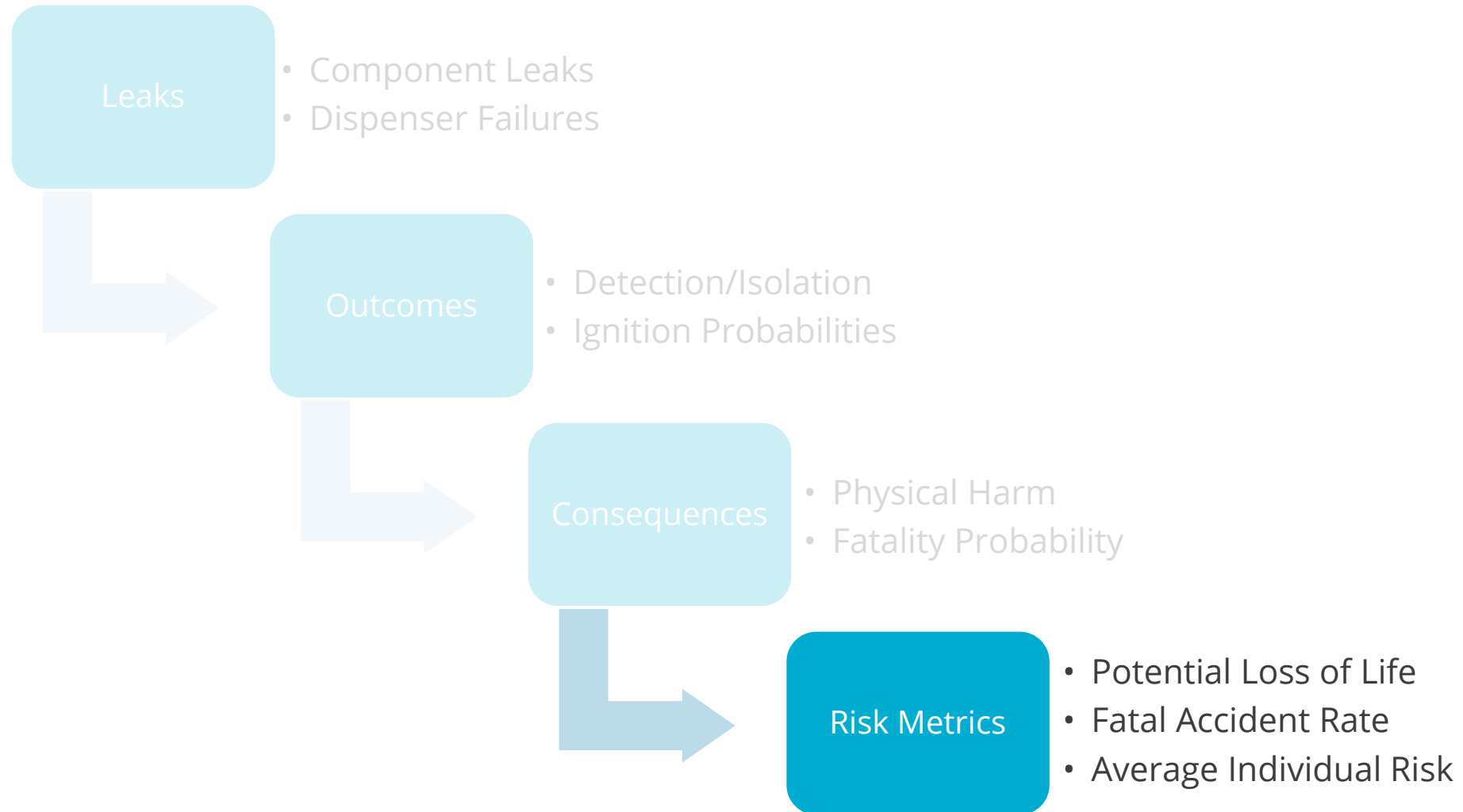
- $P(\text{fatality}) = \text{Normal CDF}(Y|\mu = 5, \sigma = 1)$

Based on peak overpressure (P_s) and impulse (i):

Model	Equation
Eisenberg – Lung Hemorrhage	$Y = -77.1 + 6.91\ln(P_s)$
HSE – Lung Hemorrhage	$Y = 5.13 + 1.37\ln(P_s \times 10^{-5})$
TNO – Head Impact	$Y = 5 - 8.49 \ln\left(\frac{2300}{P_s} + \frac{4 \times 10^8}{P_s i}\right)$
TNO – Structure Collapse *	$Y = 5 - 0.22 \ln\left[\left(\frac{40000}{P_s}\right)^{7.4} + \left(\frac{460}{i}\right)^{11.3}\right]$

* default

Overview of Risk Calculations in HyRAM+



Overall Risk Metrics



Potential Loss of Life (PLL [fatalities/year]) for n scenarios:

- $PLL = \sum_n f_n c_n$
- Each scenario is a leak size/outcome combo (e.g., 1% leak size resulting in a jet fire)

Fatal Accident Rate (FAR [fatalities/100 million hours]):

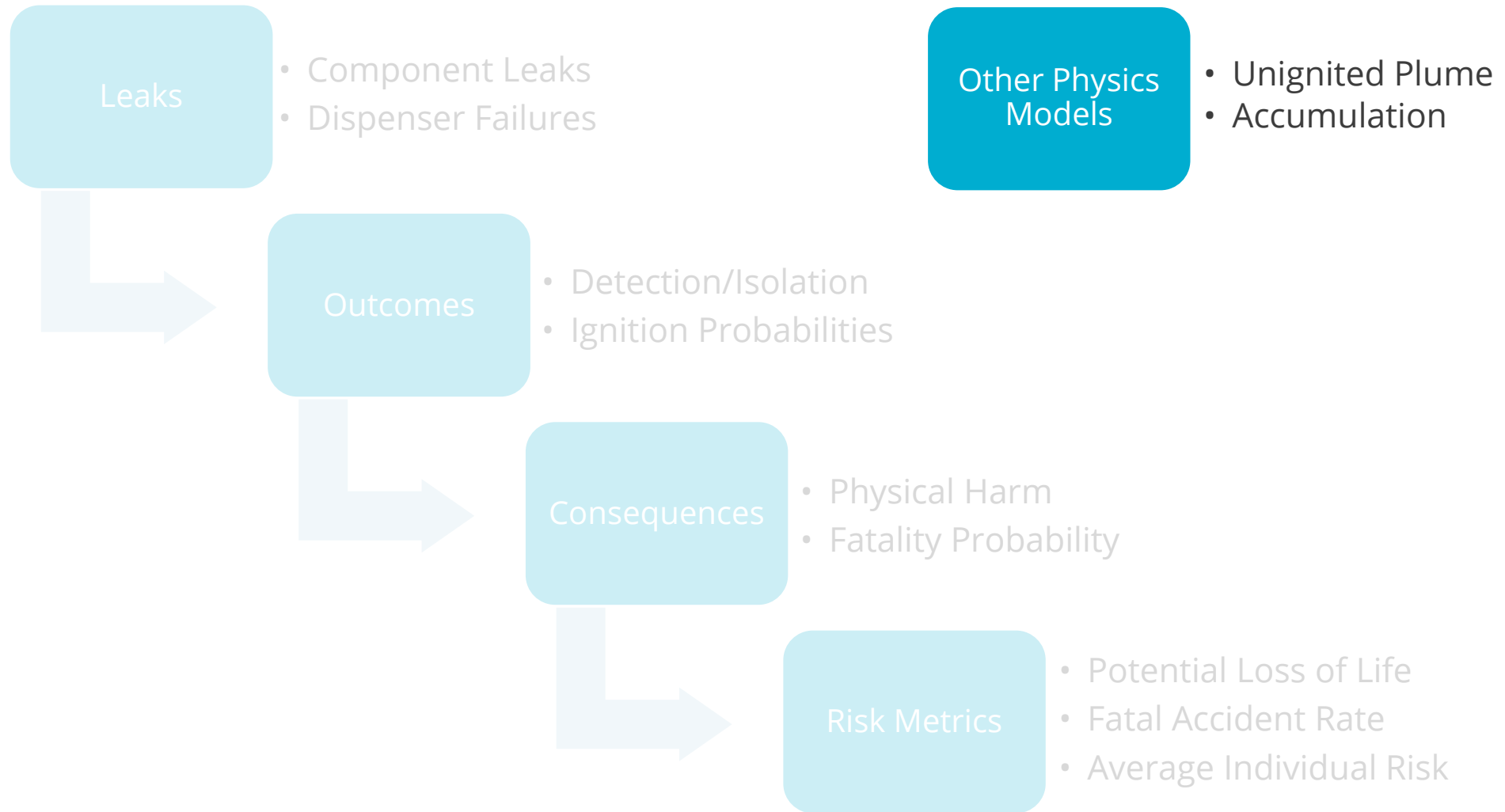
- $FAR = \frac{PLL \times 10^8}{N_{pop} 8760 \frac{hours}{year}}$
- N_{pop} is the number of people in the population considered

Average Individual Risk (AIR [fatalities/year per person]):

- $AIR = H \times FAR \times 10^{-8}$
- H is the number of exposed hours per year

Can also calculate cut sets (expected leaks for each component, branch line probabilities, etc.)

Additional HyRAM+ capabilities



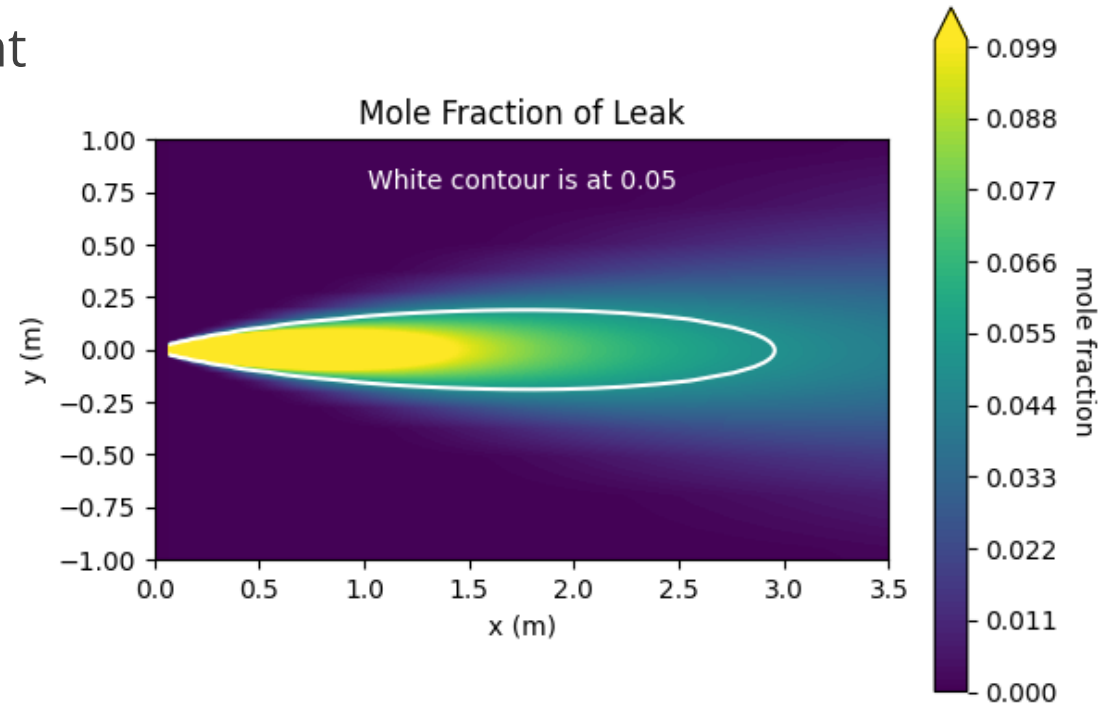
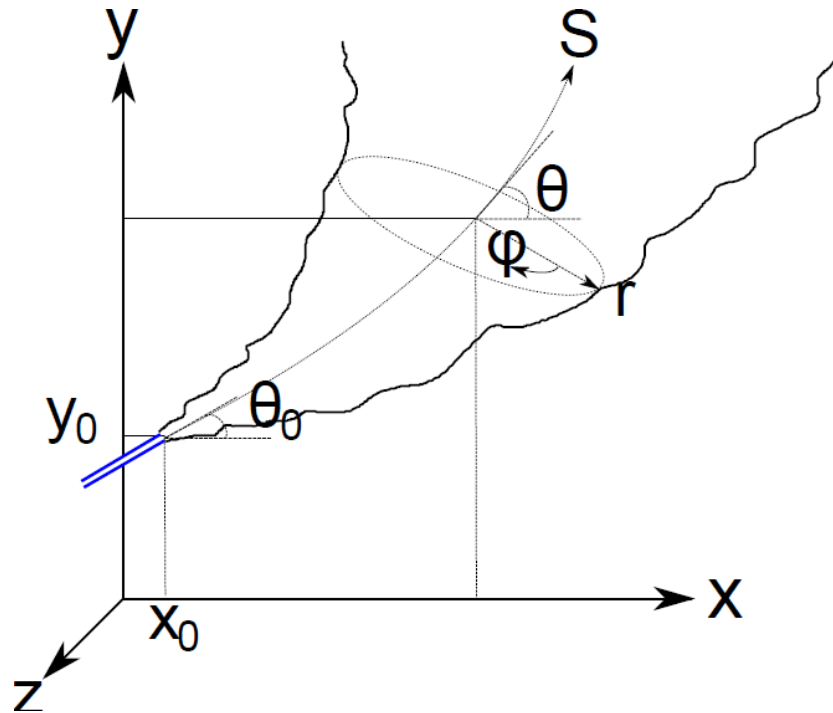
Physics Models – Jet Plume Dispersion



1-D Reduced Order Model

Leak size, conditions; surrounding environment

Useful for concentration contours



Physics Models – Overpressure/Accumulation

1-D accumulation model of a leak inside an enclosure

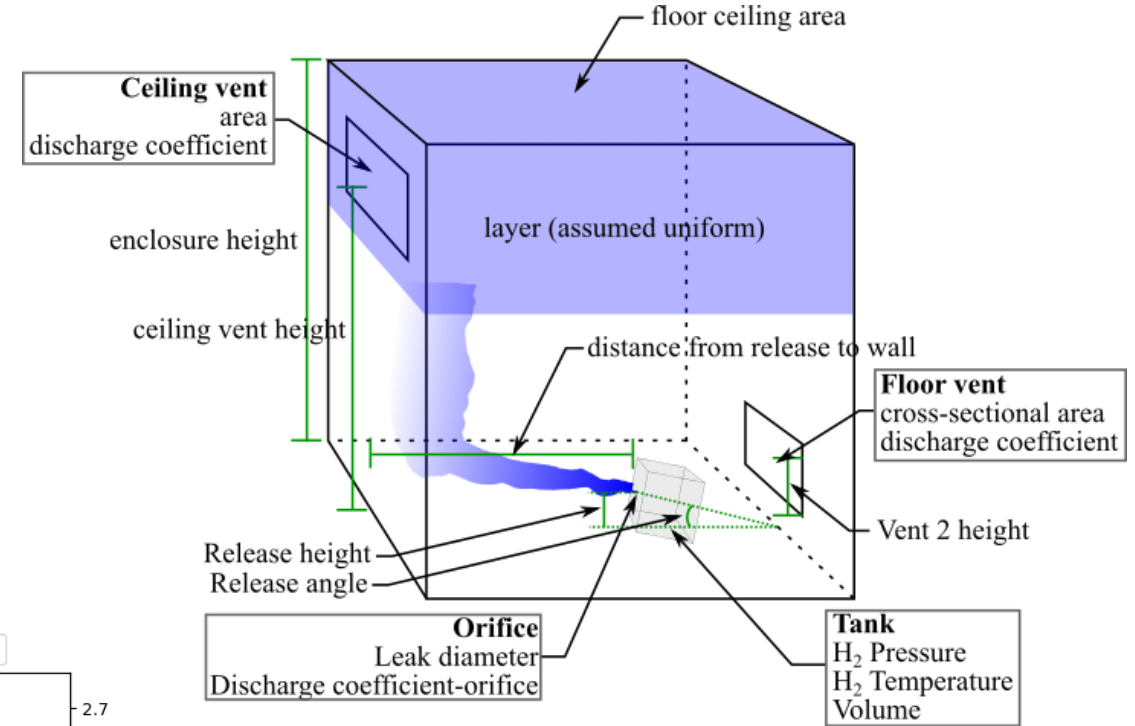
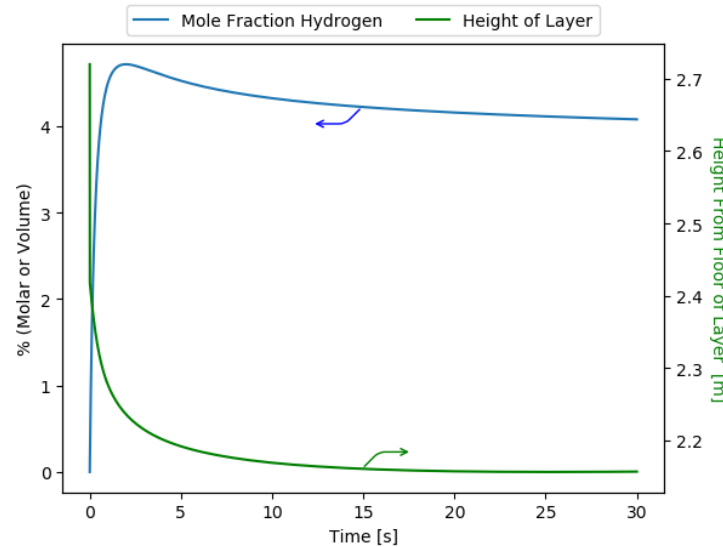
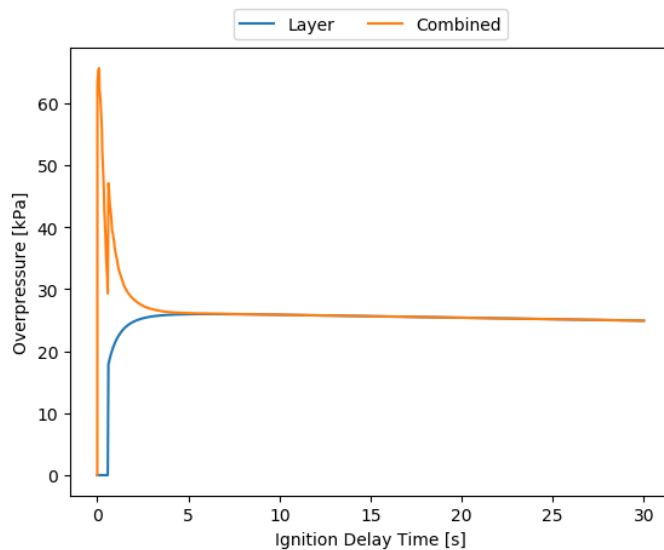
- Tracks concentration of plume and uniform layer

Assumes ceiling layer is uniform concentration

Flammable mass for plume and layer based on upper and lower flammability limits

Overpressure is peak overpressure if plume/layer were to ignite after some delay

- Not an overpressure history plot





Modification and Validation of Risk and Consequence Models for LNG (Liquid Methane)



Validation with Cryogenic Methane Releases



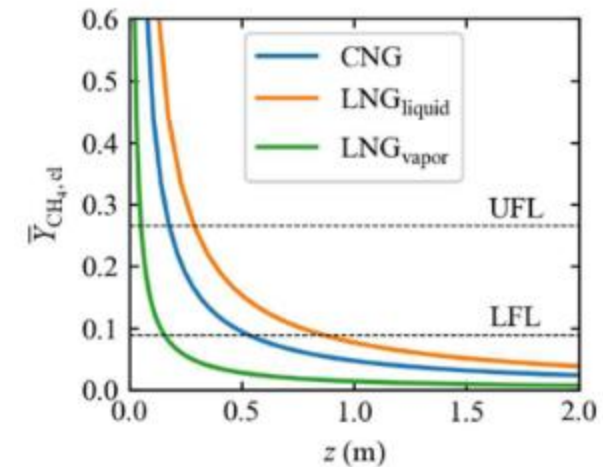
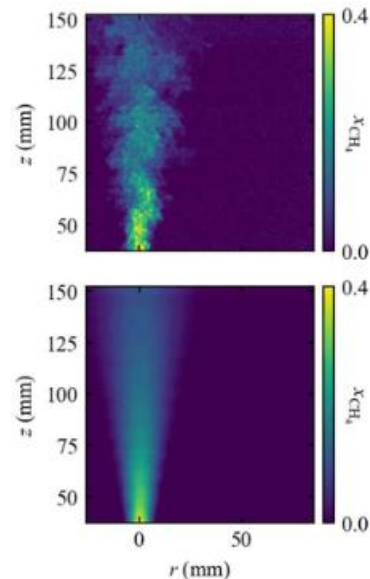
Prior work done for DOE VTO (2018)

Data collected from Raman scattering images of liquid and near liquid methane

Measured methane concentrations compared to empirical relationships for warm gas releases

- In agreement in terms of centerline concentration decay rate, self-similarity, and half-width decay rate

d_{noz} (mm)	P_{noz} (bar _{abs})	T_{noz} (K)	n_{heights}	T_{exit} (K)	P_{exit} (bar _{abs})	ρ_{exit} (kg/m ³)	V_{exit} (m/s)
1.00	2.0	128	1	112	1.07	1.93	272
1.00	2.0	179	6	153	1.08	1.38	323
1.00	2.0	187	1	160	1.08	1.32	330
1.00	2.0	219	1	188	1.08	1.12	358
1.00	5.0	139	5	125	2.63	4.53	280
1.00	6.0	147	6	128	3.22	5.36	282
1.25	2.0	164	5	140	1.08	1.52	308
1.25	2.5	126	11	115	1.31	2.38	274
1.25	3.0	129	6	117	1.57	2.82	276
1.25	4.0	133	11	121	2.09	3.69	278
1.25	5.0	137	6	125	2.61	4.55	280
1.25	6.0	143	7	128	3.16	5.38	282



Leak frequencies are uncertain but necessary for risk analysis



- Per-component annual leak frequencies can be applied broadly to facilities of different sizes and types
- Can propagate leak frequencies through risk models to predict the frequency of risk-significant events
- Many sources of uncertainty affect our ability to estimate leak frequencies

Aleatory uncertainty: inherent variation between the designs, materials, maintenance, operating conditions, ages, etc. of different components

Epistemic uncertainty: lack of data for new systems, lack of reporting or inconsistent reporting for existing systems, measurement errors

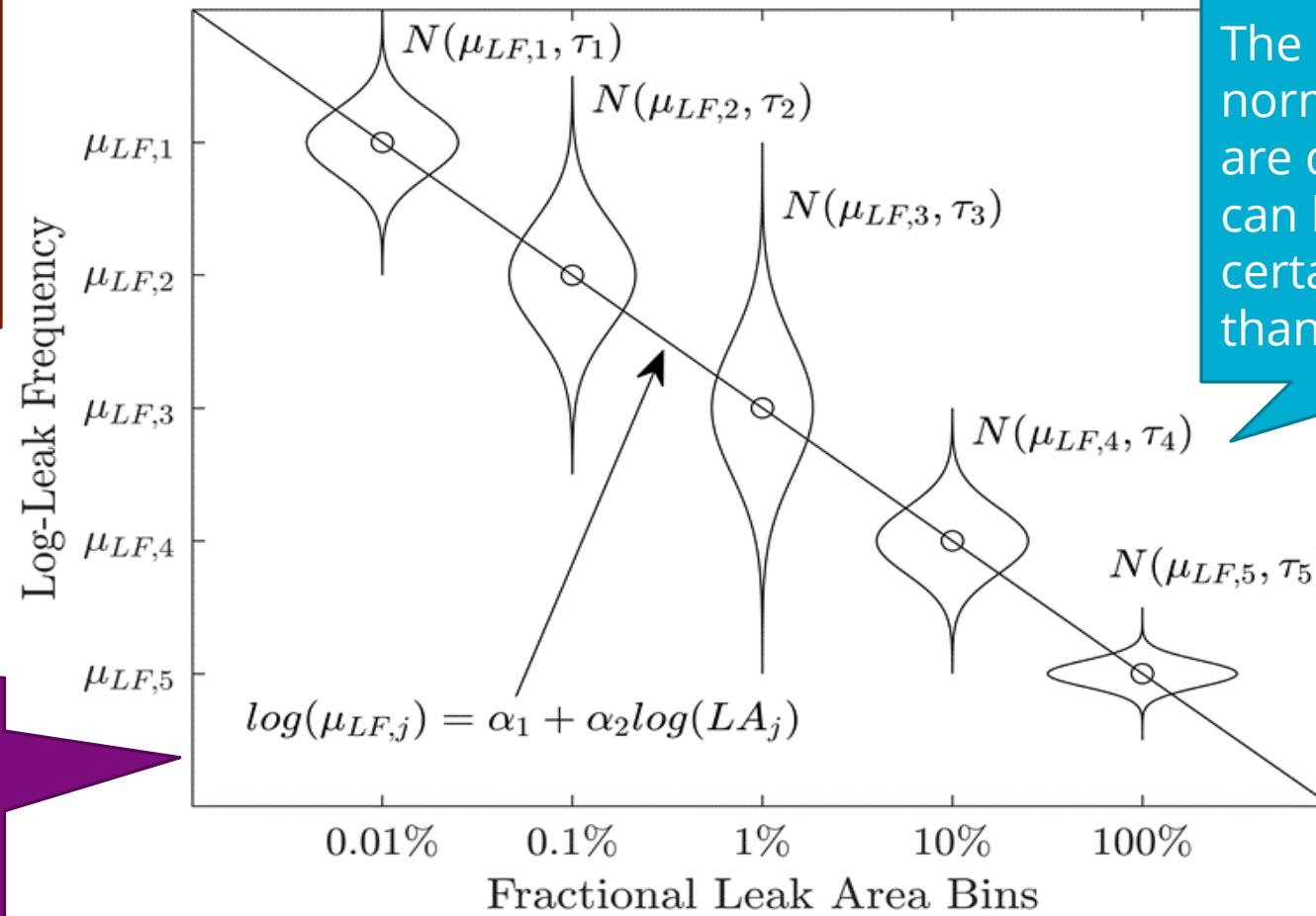
Bias: from detection (larger leaks are easier to detect), reporting requirements

Prediction model should include state-of-knowledge uncertainties that may be reduced over time with more data, but should also include the within-population variation

Model estimates leak frequencies for each fractional leak area using distributions that are related by their means



Distributions are fit in log-space, so $\mu_{LF,1}$ is the mean of the normal distribution on the log-leak frequency for the smallest leak size bin



The precisions of the normal distributions are different so there can be higher certainty in some bins than in other bins

The linear relationship between means allows data from one bin to influence other bins that may have little or no data

May be insufficient data to draw reliable conclusions about leak frequencies for hoses and joints

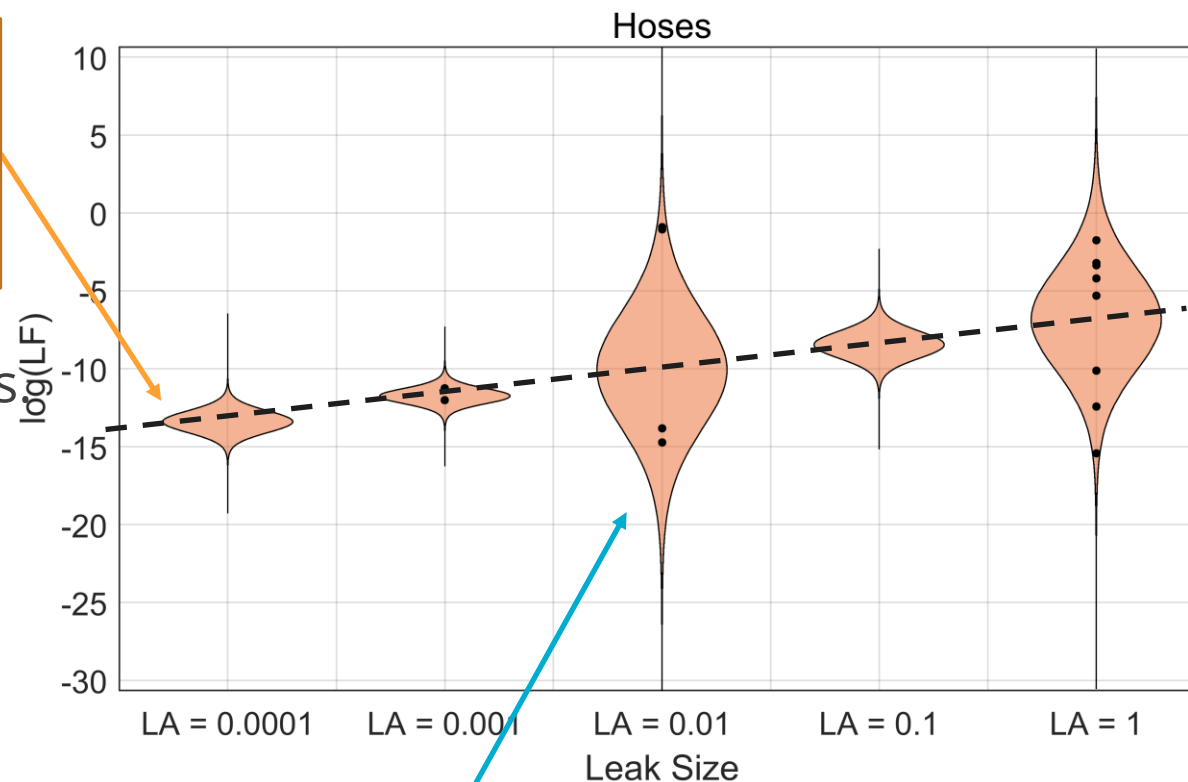


Linear relationship indicates similar or higher frequencies for large leaks compared to small leaks; it is unclear if this is due to lack of data or physics related to hoses

Violin plot shows the distribution of results
This:

- gives more detail than a mean or median with uncertainty bounds,
- emphasizes the normal distribution assumption, and
- discourages interpolation between the discrete leak size bins.

Estimates span multiple orders of magnitude; hose estimates can be very high for some leak sizes



The data we have may not be consistent with the assumed normal distribution, but need more data to know

The highest estimated median leak frequencies were uniquely high for joints in the LNG analysis



Component	Leak Size	5th	Median	95th	Component	Leak Size	5th	Median	95th
Flange	0.01%	1.13E-05	4.18E-05	1.14E-04	Pipe	0.01%	3.08E-07	2.67E-06	2.30E-05
	0.1%	3.52E-06	2.26E-05	1.82E-04		0.1%	1.39E-07	1.44E-06	1.52E-05
	1%	2.84E-07	1.40E-05	7.14E-04		1%	1.17E-07	7.86E-07	5.22E-06
	10%	8.81E-08	8.68E-06	7.30E-04		10%	4.59E-08	4.25E-07	3.91E-06
	100%	4.03E-08	5.24E-06	5.40E-04		100%	1.15E-08	2.30E-07	4.63E-06
Heat Exchanger	0.01%	5.41E-04	2.34E-03	1.22E-02	Valve	0.01%	2.40E-05	8.43E-05	2.48E-04
	0.1%	1.03E-04	8.93E-04	7.27E-03		0.1%	8.76E-06	4.20E-05	2.18E-04
	1%	3.11E-05	3.24E-04	3.22E-03		1%	3.54E-06	2.16E-05	1.53E-04
	10%	2.69E-06	1.17E-04	5.14E-03		10%	4.72E-07	1.18E-05	2.69E-04
	100%	3.13E-06	4.18E-05	6.27E-04		100%	2.34E-07	6.42E-06	1.29E-04
Hose	0.01%	4.49E-07	1.52E-06	5.13E-06	Vaporizer	0.01%	1.27E-04	8.19E-03	5.24E-01
	0.1%	3.16E-06	7.89E-06	1.99E-05		0.1%	1.24E-03	2.63E-02	5.57E-01
	1%	4.38E-08	4.13E-05	3.82E-02		1%	1.15E-02	8.46E-02	6.23E-01
	10%	4.65E-05	2.14E-04	1.00E-03		10%	8.65E-02	2.72E-01	8.57E-01
	100%	2.96E-06	1.10E-03	4.34E-01		100%	2.79E-01	8.75E-01	2.75E+00
Joint	0.01%	9.89E+02	3.51E+04	1.25E+06	Vessel	0.01%	8.18E-05	4.77E-04	3.41E-03
	0.1%	3.20E+01	4.77E+02	7.09E+03		0.1%	3.69E-06	1.39E-04	5.25E-03
	1%	9.98E-01	6.46E+00	4.18E+01		1%	1.65E-06	3.90E-05	9.14E-04
	10%	2.78E-02	8.76E-02	2.76E-01		10%	2.03E-07	1.10E-05	5.80E-04
	100%	4.32E-04	1.19E-03	3.26E-03		100%	1.67E-08	3.05E-06	5.77E-04

Median characterizes the center of the distribution but, due to the within-population variation, higher or lower percentiles may be more appropriate for specific sites.


The distributions may shift/stretch/shrink as more data become available, but will never reduce to a point-value even with perfect knowledge due to this variation.


Modification of HyRAM+ Software Models and GUI



Incorporation of modified models, physical properties into source code

Addition of fluid and phase selectors to user graphical user interface (GUI)

Fuel: 

Fluid phase: 

Re-naming and re-branding of HyRAM to HyRAM+



Publication of source code on public GitHub repository:

<https://github.com/sandialabs/hyram>



Summary, Conclusions, and Future Work



Summary and Conclusions



Reduced-order engineering models for hydrogen release behavior and risk assessment have been modified to enable the use of liquid methane

- Leveraged efforts from prior development of base models as well as CNG-related efforts
- LNG-specific leak frequency distributions have been developed to inform LNG risk assessments

Free and open source HyRAM+ (née HyRAM) released, enabling use of models and data

- Downloadable from <https://hynam.sandia.gov>
- Includes Windows installer, link to source code repository, and Technical Reference Manual documentation [task deliverable]

Next Steps/Current Efforts



Updates to gaseous and liquid hydrogen ignition probabilities [DOE HFTO]

- Could identify how LNG ignition frequencies may differ from CNG

Incorporation of unconfined overpressure model into risk calculations [DOE HFTO]

- Minimize need for external calculations

Addition of cryogenic liquid hydrogen pooling model [DOE HFTO]

- Flammable cloud could form above evaporating pool
- Same model could be utilized for liquid methane or LNG releases

Use of mixtures as source fluid rather than pure fluid [DOE HFTO, DOE VTO]

- Useful for natural gas or propane mixtures, rather than pure methane or propane as a proxy
- Can be used to assess safety for hydrogen-natural gas blends



Thank you!

Questions?

Brian Ehrhart bdehrha@sandia.gov

Final Reports Available: <https://hynam.sandia.gov>



Backup Slides



Leak Frequency Model



Hierarchical probability distribution model

LF_j is the annual leak frequency for a component for a leak size j

- Lognormal probability distribution

Parameters themselves are distributed as probabilities

$$\log(LF_j) \sim N(\mu_{LF,j}, \tau_j)$$
$$\log(\mu_{LF,j}) = \alpha_1 + \alpha_2 \log(LA_j) \quad \tau_j \sim \text{Gamma}(r_j, s_j)$$
$$\alpha_1 \sim N(\alpha_{11}, \alpha_{12}) \quad \alpha_2 \sim N(\alpha_{21}, \alpha_{22})$$

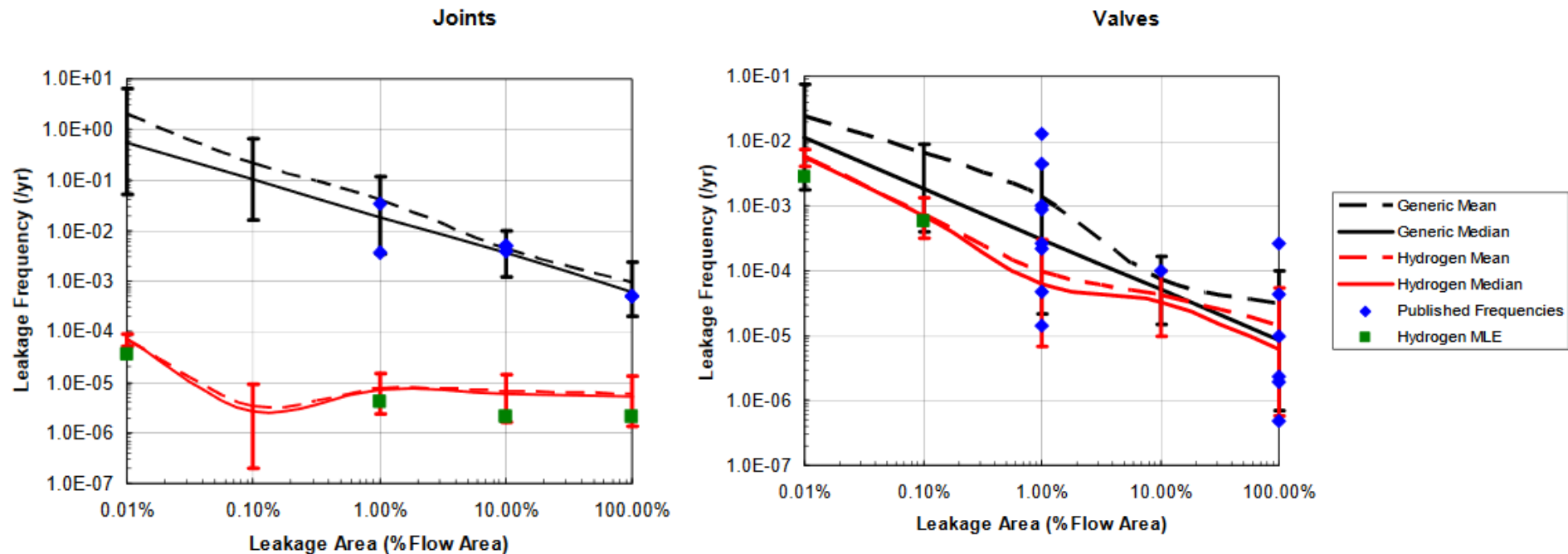
Gaseous Hydrogen Leak Frequencies in HyRAM+



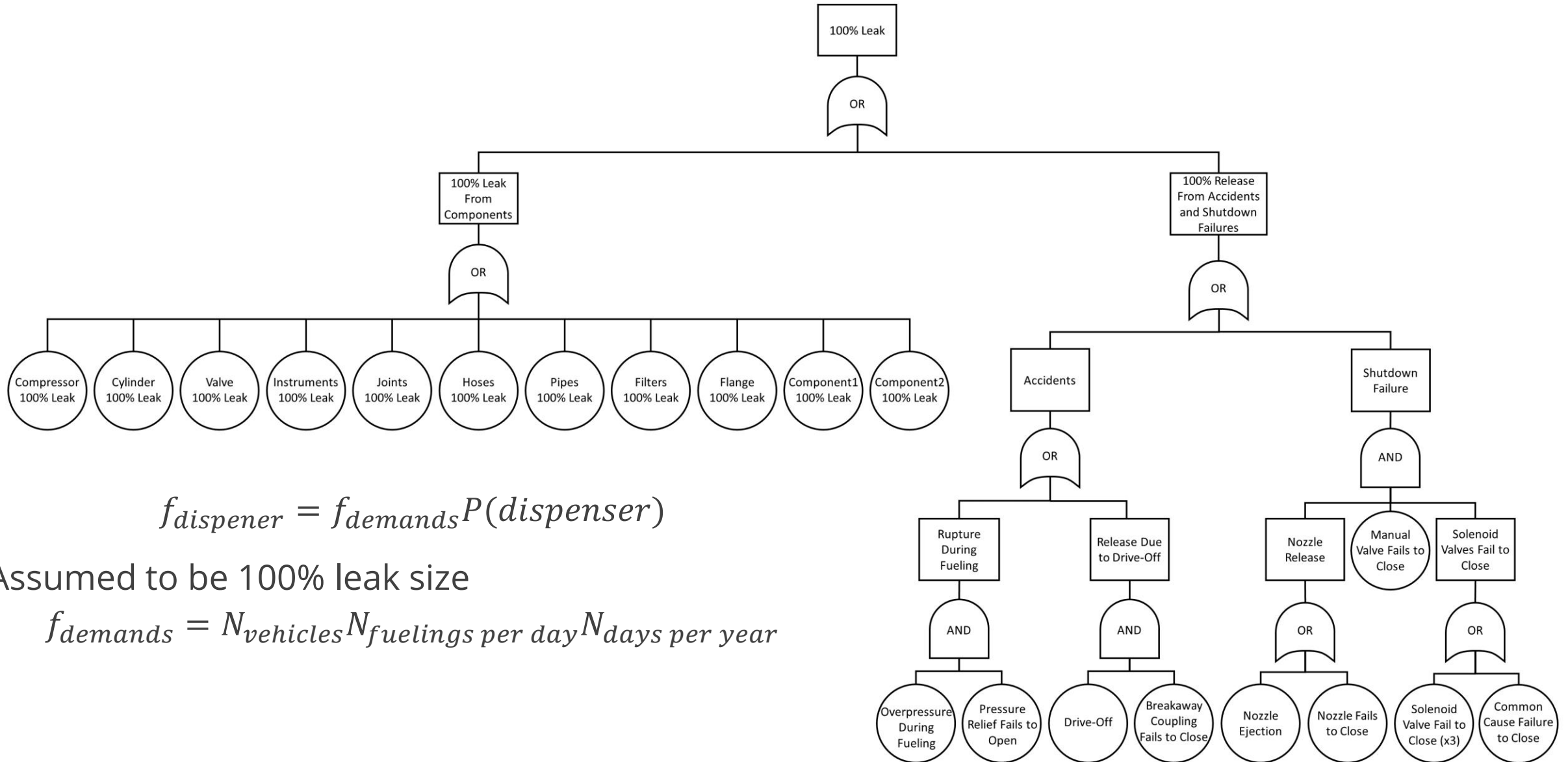
From: LaChance, et al. "Analyses to Support Development of Risk-Informed Separation Distances for Hydrogen Codes and Standards" SAND2009-0874, March 2009

Use of generic leak frequencies from oil & gas industry

Updated with hydrogen-specific data



Dispenser Failure Fault Tree



Physics Models – Jet Flame

1-D Reduced order model

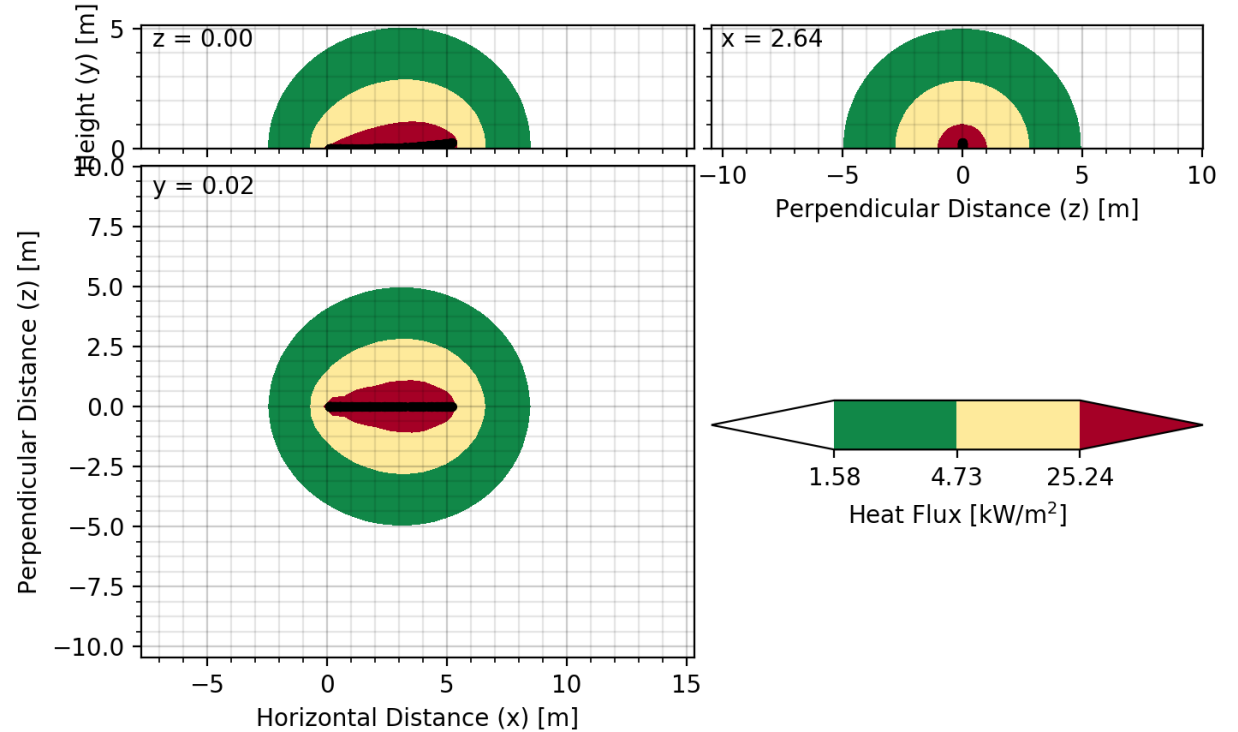
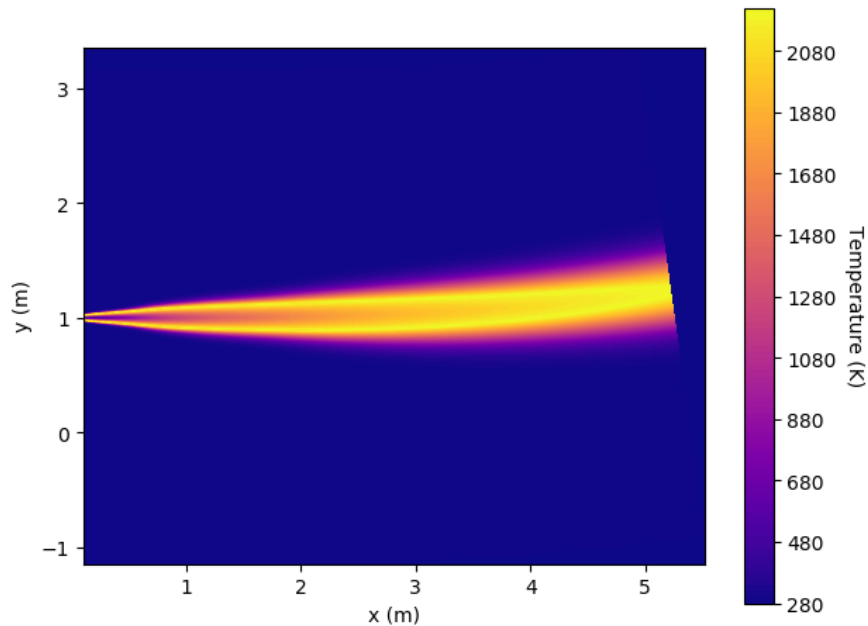
- Similar to jet plume

Multi-point radiation calculations

Temperatures (up to visible flame length)

Heat flux contours

- Also at specific positions



Model Descriptions – Blast Curves



- TNT Equivalence

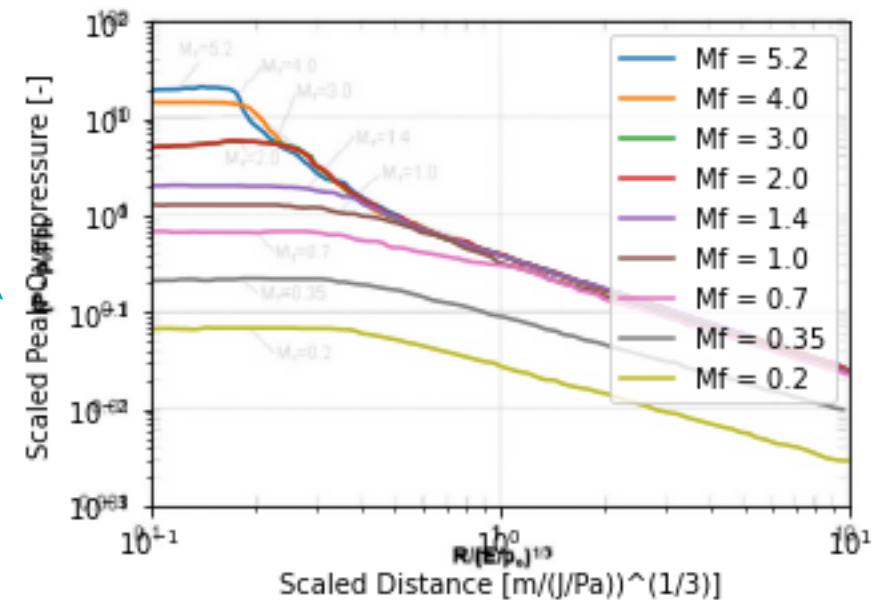
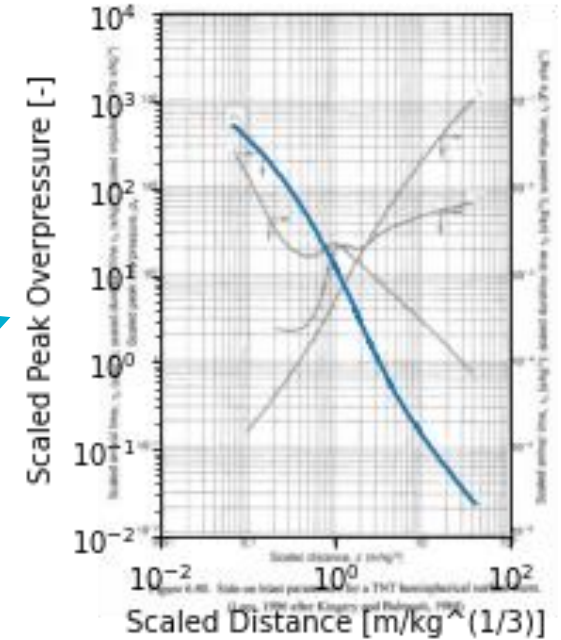
- Calculate equivalent mass of TNT: $W_{TNT} = \alpha_e \frac{W_f H_f}{H_{TNT}}$
- Calculate scaled-distance: $\bar{R} = \frac{R}{W_{TNT}^{1/3}}$
- Read scaled-overpressure (or impulse) from plot

- Baker-Strehlow-Tang (BST)

- Calculate scaled-distance: $\bar{R} = \frac{R}{(E/P_0)^{1/3}}$
- Read scaled-overpressure (or impulse) from plot
 - Based on flame speed

- Bauwens and Dorofeev

- Calculate detonation cell size based on equivalence ratio throughout plume
- Calculate detonable mass based on cell size gradient
- Calculate scaled distance: $R^* = \frac{R p_0^{1/3}}{E^{1/3}}$
- Calculated scaled overpressure: $P^* = \frac{0.34}{(R^*)^{4/3}} + \frac{0.062}{(R^*)^2} + \frac{0.0033}{(R^*)^3}$



The model is implemented as a trivial Bayesian hierarchical model that is updated in stages



Initial values are provided for $\alpha_{11}, \alpha_{12}, \alpha_{21}, \alpha_{22}, \tau_j$
 These values are calibrated using data and the definitions at the bottom of the hierarchy

$$\alpha_1 \sim \text{normal}(\alpha_{11}, \alpha_{12})$$

$$\alpha_2 \sim \text{normal}(\alpha_{21}, \alpha_{22})$$

$$\tau_j \sim \text{gamma}(s_j, r_j)$$

First (and last) level in hierarchy

$$\log(\mu_{LF,j}) = \alpha_1 + \alpha_2 \log(LA_j) \quad \log(LF_j) \sim \text{normal}(\mu_{LF,j}, \tau_j)$$

Base model that is assumed to govern published leak frequencies

Once the values for $\alpha_{11}, \alpha_{12}, \alpha_{21}, \alpha_{22}, \tau_j$ are calibrated, the model is implemented by sampling from the top of the hierarchy, propagating to the bottom, and exponentiating the final estimate. The update process can be repeated many times to include different data sets.