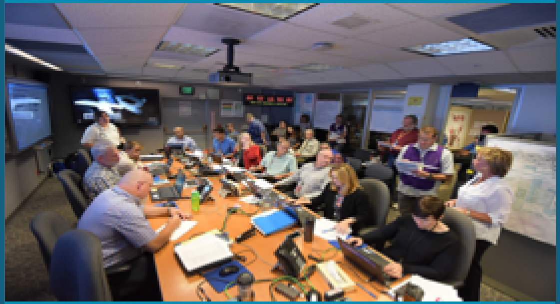
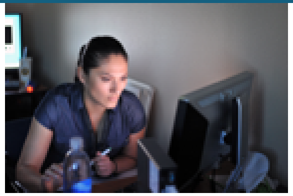
May 11, 2021

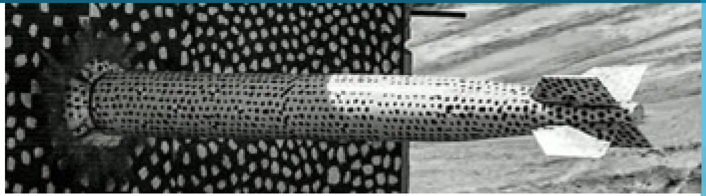
Sandia National Laboratories

SAND2021-6106C

A Computational Scenario Based Assessment of Hydrogen Isotope (^{3}H) Fire Safety







For the 12th US National Combustion Institute Meeting, May 26-30, 2021

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Fire Science and Technology Department

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Fire Science & Technology

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SAND2021-???? C

Introduction

Tritium is an isotope of Hydrogen (^3H) useful as a tracer, used in lighting, and in physics experiments

Sandia has low quantities of sub-atmospheric tritium (~1 gram), yet federal guidelines may mandate significant protocol costs if safety regulations are not precise

- This work aims to provide basis for consideration of a more precise or lenient conversion assumption than the conservative approximation of 100% or 50% for a facility fire

Unlike protium (^1H), tritium is most hazardous to humans as water (T_2O or THO)

- Historical hydrogen (^1H) safety studies are focused elsewhere (jetting fires, explosions)
- For tritium, the key to understanding the hazard is the reaction of the trace release
- The human body metabolizes water, whereas T_2 does not appreciably penetrate skin (Mishima and Steele, 2002)

Because of the hazard and low tritium inventories, computational studies of hazards are ideal

- Problem #1 is that there are few sources for physical properties and fire performance for tritium
- Problem #2 is that computational tools require verification and validation for credibility
- Problem #3 is that there are a near infinite combination of scenarios of potential interest

ISO-9705

The fire community has a corner fire standard for assessing flammability under representative conditions

- Involves a 100 kW fire in a back corner
- After 10 minutes (optional) increase to 300 kW
- Designed to mimic a waste basket fire

We seek to leverage this 'standard' for tritium safety

- Release of 0.1 g of tritium in the opposite corner
- Primary performance parameter of interest is the conversion of T_2 to T_2O

Since tritium is hazardous and expensive, it will be done computationally

- Little to nothing has been done previously on the dynamics of a tritium fire accident either experimentally or computationally
- This work is intended to help fill this gap

Geometry from the standard

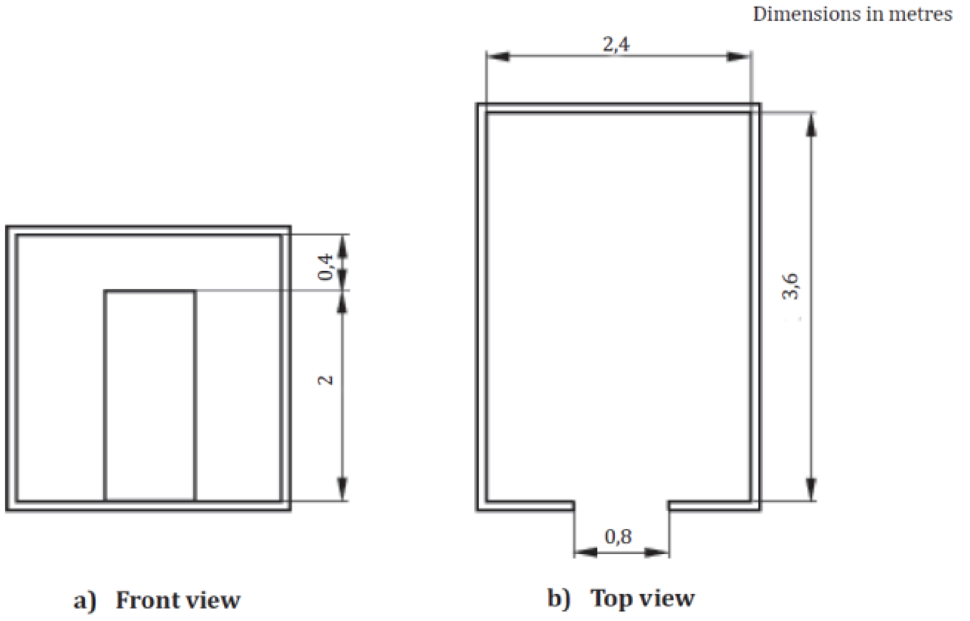
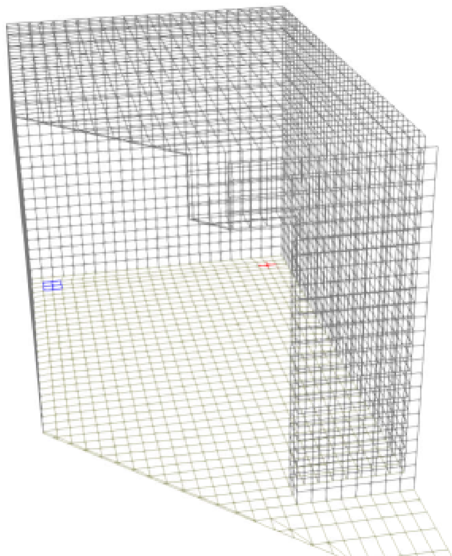


Figure 1 — Fire test room

The Coarse Mesh



Computational Methods

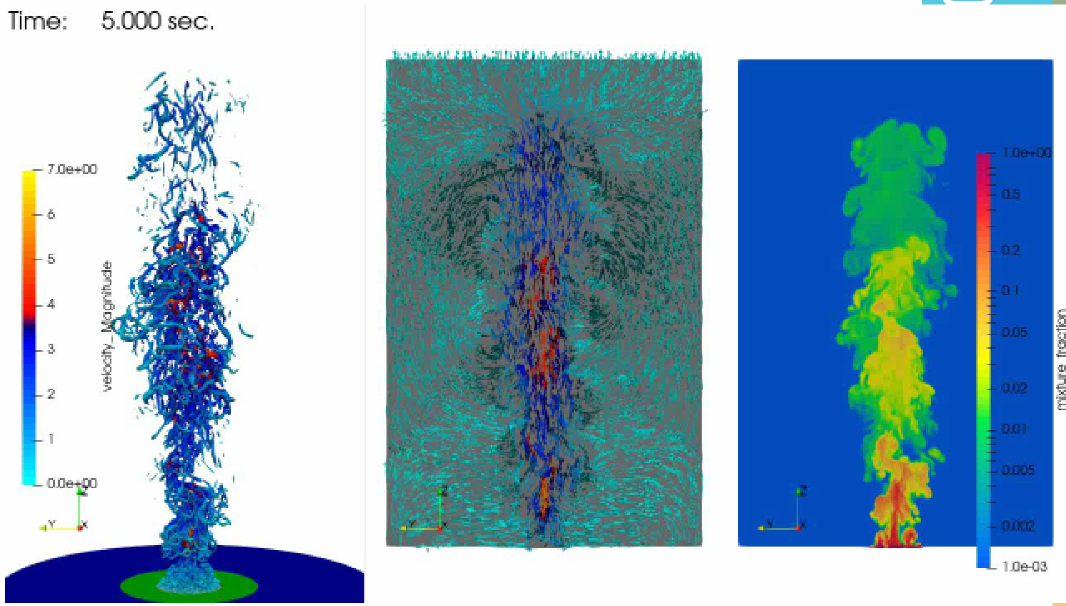
SIERRA/Fuego is Sandia's unstructured low-Mach reacting flows code for simulating fires

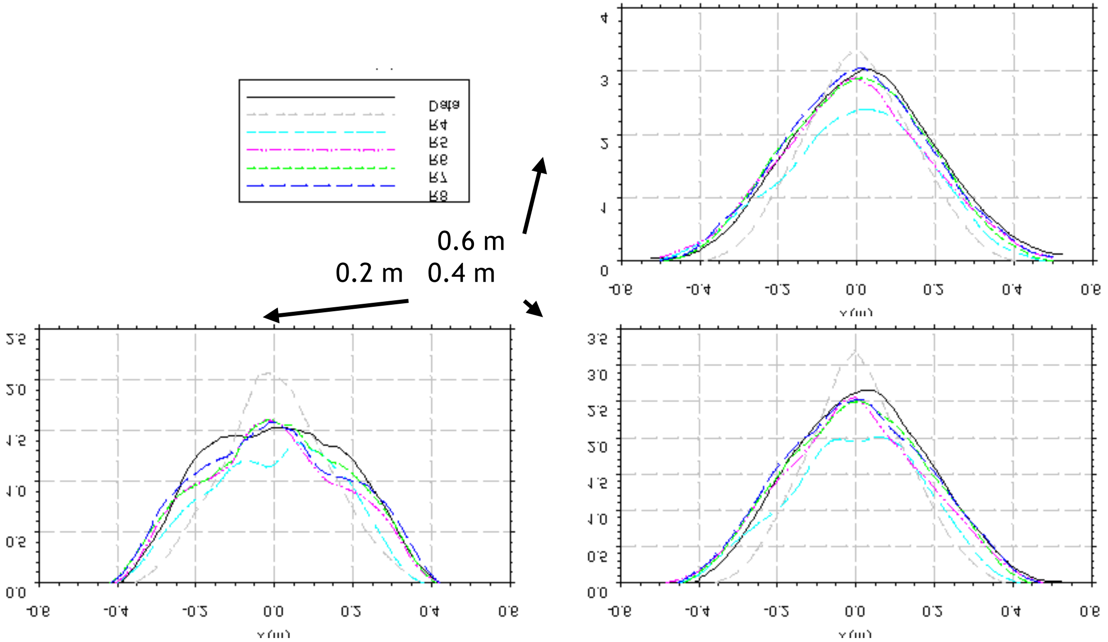
- Verification credibility stems from version control and nightly regression testing as per DOE O 414.1D
- Validation credibility comes from a myriad of historical test problems (He plume results illustrated on right)

Simulation parameters for this study:

- Hybrid LES/RANS TFNS turbulence
- EDC reactions for corner fire
- Marinov et al. (1995) 1 step H_2 kinetic rate fo reaction of trace gas: $k_{global} = A exp(-E/R\,T)[H_2]^{1.0}[O_2]^{0.5}$
- Hex mesh with 3 levels of refinement
- Discrete Ordinates for radiation, gray assump
- 1D conducting walls

<u>Example He plume validation results</u>:





Simulation Matrix

Anticipating continuing lack of T_2 validation data, we also include other isotopes for simulations

- Endeavoring to understand how well ^{1}H and ^{2}H can function as surrogates for ^{3}H

Initial 100 kW fires resulted in very low conversion

- 300 kW was promoted to ‘baseline’ conditions to simulate behavior in a more dynamic regime

Simulation matrix covers a variety of factors:

- Mesh resolution to understand spatial convergence
- Kinetic and Schmidt number variations to assess the importance of the reaction rate and diffusion parameters to the results

Tritium release distance from the fire was also varied

Case	Mesh	Power	Contaminant	Other Variables
1-C3T	Coarse	300 kW	T_2	
2-M3T	Medium	300 kW	T_2	
3-F3T	Fine	300 kW	T_2	
4-M3D	Medium	300 kW	D_2	
5-M3H	Medium	300 kW	H_2	
6-M3TA1	Medium	300 kW	T_2	Kinetic pre-exponential (A) parameter reduced by a factor of 10
7-M3TA2	Medium	300 kW	T_2	Kinetic pre-exponential (A) parameter reduced by a factor of 3.16
8-M1H	Medium	100 kW	H_2	
9-M1D	Medium	100 kW	D_2	
10-M1T	Medium	100 kW	T_2	
11-M1DS1	Medium	100 kW	D_2	Schmidt number reduced from 0.7 to 0.475
12-M1DS2	Medium	100 kW	D_2	Schmidt number reduced from 0.7 to 0.2
13-M3T25	Medium	300 kW	T_2	Release inlet 25% of nominal distance from fire
14-M3T50	Medium	300 kW	T_2	Release inlet 50% of nominal distance from fire
15-M3T75	Medium	300 kW	T_2	Release inlet 75% of nominal distance from fire
16-M2T	Medium	200 kW	T_2	

Mesh	Nominal Spacing (cm)
Coarse	8.5
Medium	4.2
Fine	2.5

Temporal Details and Results Scheme

Fire was started at t=0

Contaminant ^nH release was constant from 10-16 seconds

Dynamics were tracked until at least 3 minutes

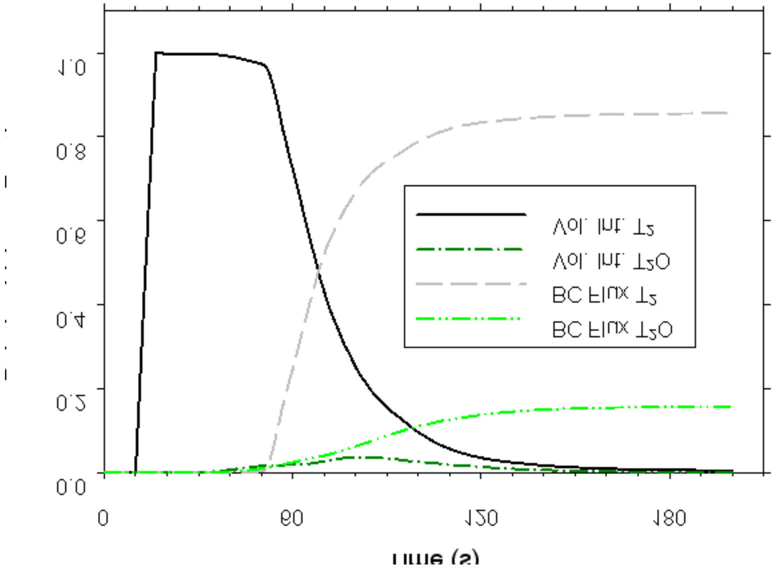
We integrate the volume fraction to obtain fractional conversion in the system (as illustrated in right, top figure)

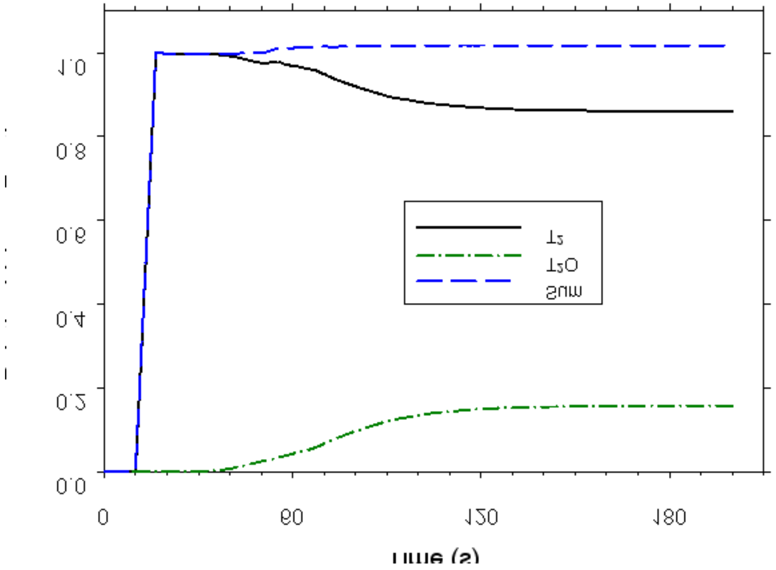
- We focus on the max $(H_2O/(H_2+H_2O))$, called C1

We combine that with an integration of the mass leaving the system for total conversion (right top and bottom)

- The integration was done in the post-processor, which lacked the temporal resolution of the simulations to save on disk space
- Results are consequently approximate to a few %
- For these results C2 is the final $(H_2O/(H_2+H_2O))$

Example 2-M3T (baseline) results:

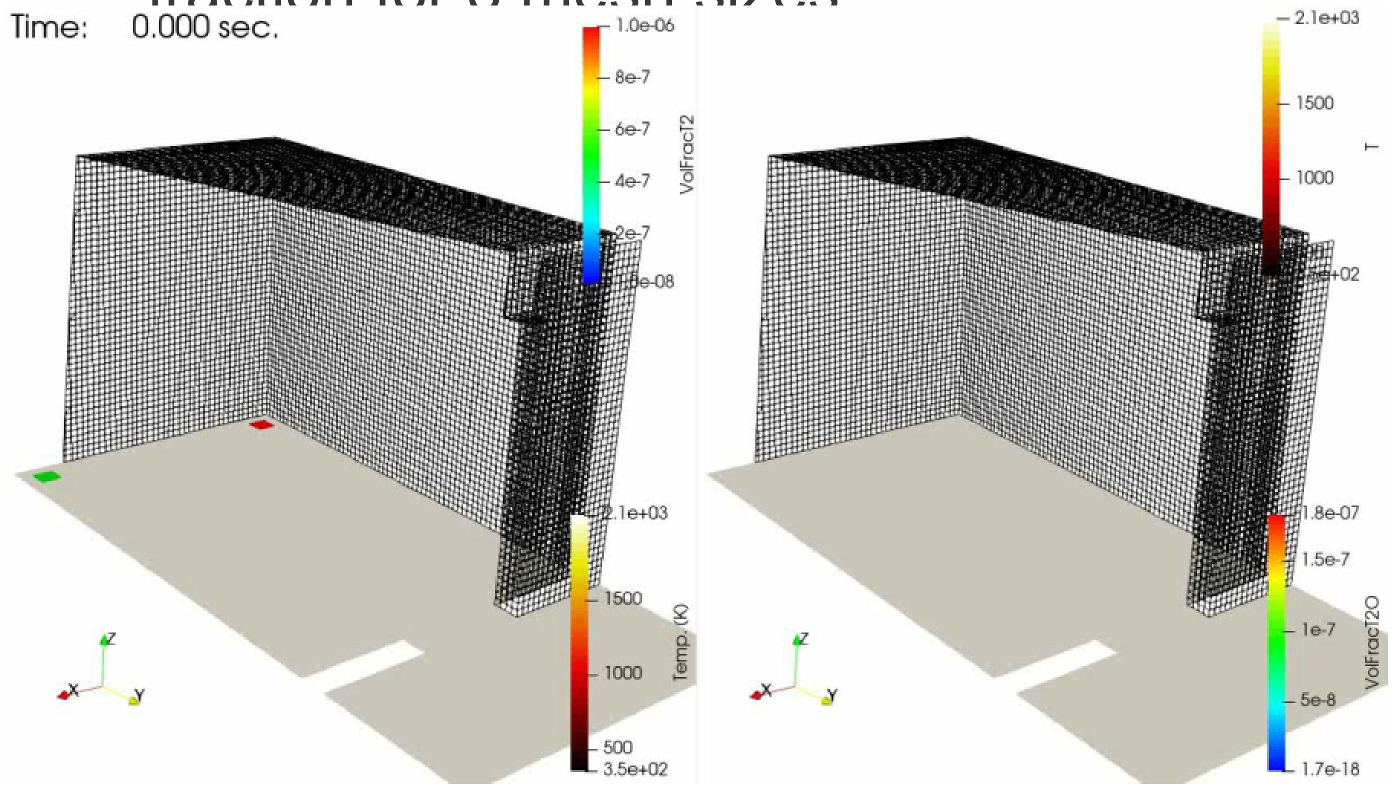


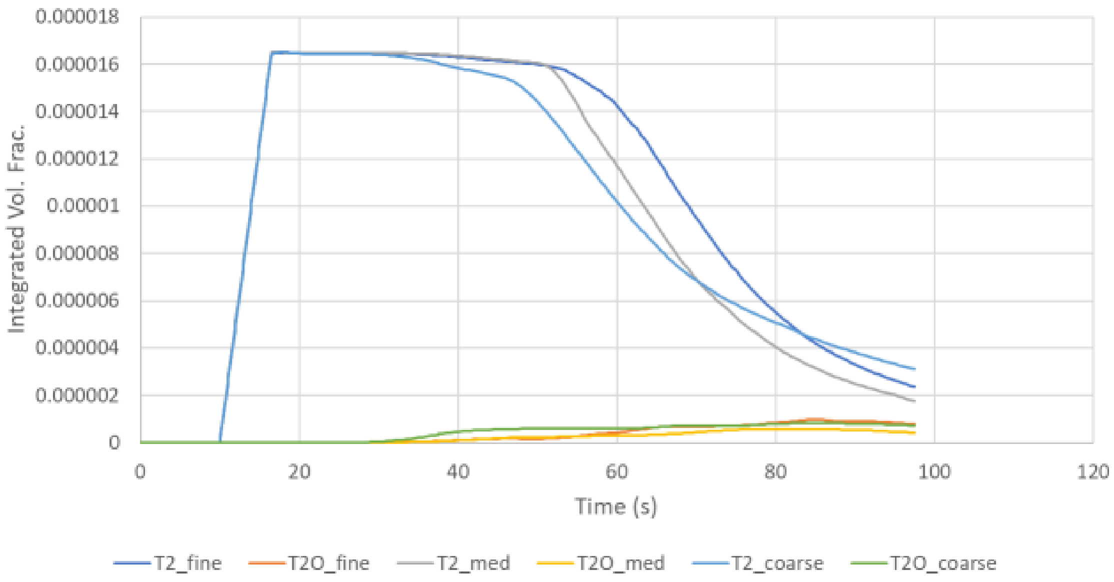


Mesh Convergence and Baseline (2-M3T) Video

Full mesh convergence was not expected, and perhaps had more effect than anticipated

Plot on right shows integrated volume fraction for 3 mesh sizes





Movie on left illustrates dynamics

Left frame has isocontours of T_2

Right frame has identical in magnitude isocontours of T_2O

Prime Results Table

Table on the right highlights principal results

Except for case 13,14, C1 never exceeds 0.1

C2 results frequently < 0.1

Schmidt number (11, 12) and kinetic rate (6, 7) exhibited small (negligible) effect

Three parameters exhibited largest effect:

- Isotope
- Power parameter for fire
- Distance from the fire of the release

CASE	C1	T1 (S)	C2	T2 (S)
1-C3T	0.0513	86	0.309	180
2-M3T	0.0348	84	0.1543	180
3-F3T*	0.0595	85	0.2534	180
4-M3D	0.0447	74.5	0.195	180
5-M3H	0.0974	57.5	0.388	180
6-M3TA1	0.0397	81	0.1628	180
7-M3TA2	0.0384	82.5	0.1634	180
8-M1H	0.0067	70.0	0.0322	180
9-M1D	0.0054	121	0.0264	180
10-M1T	0.0087	113	0.0374	180
11-M1DS1	0.0052	125	0.0281	180
12-M1DS2	0.0051	116.5	0.0252	180
13-M3T25	0.9063	19.3	1.0	180
14-M3T50	0.3601	29.5	0.6159	180
15-M3T75	0.0520	82	0.2224	180
16-M2T	0.0463	62	0.2124	180

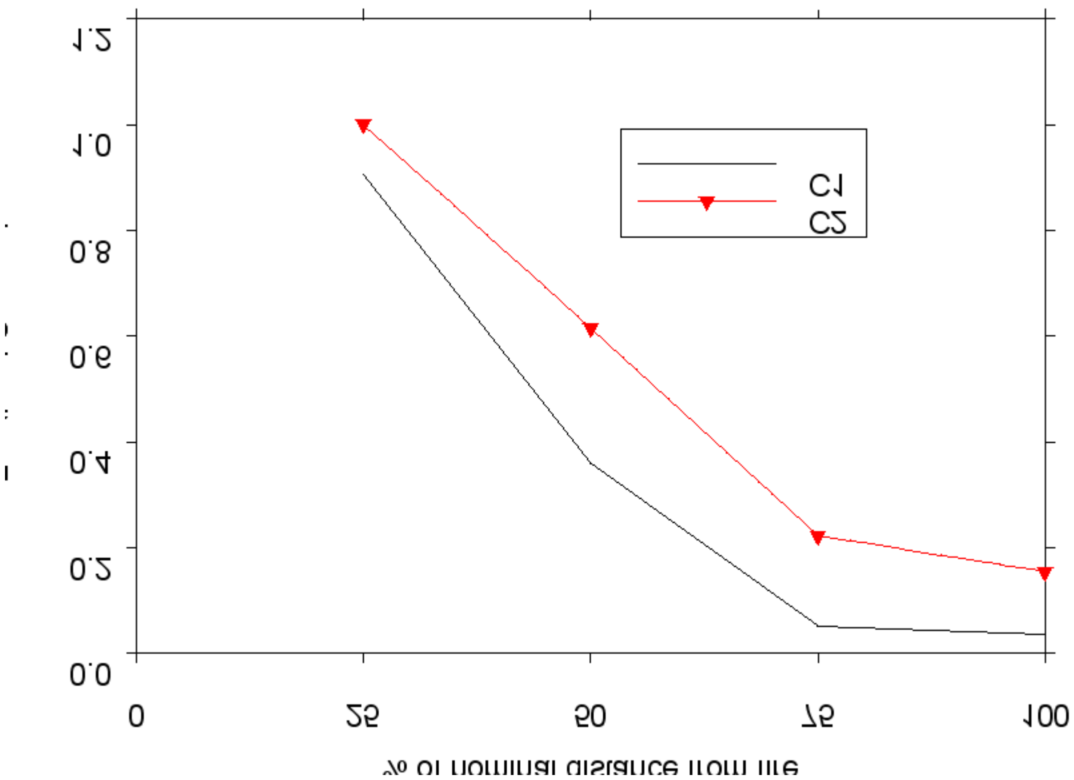
* fine results incomplete for C2, T2

Recent final results

Distance From Fire

Plot on right shows significant drop in fractional conversion for 50% nominal distance, or about 1 m away from fire

100% conversion at 25% nominal distance from the fire (close)

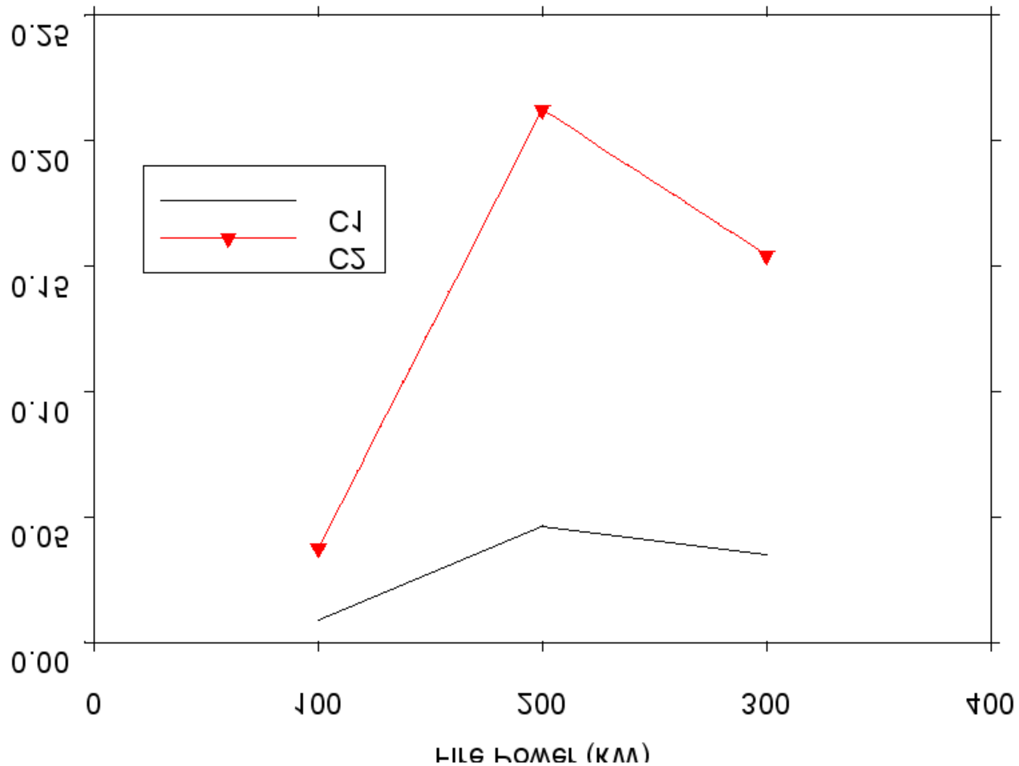


Fire Power Effect

Plot on right shows non-monotonicity of trends

- No satisfactory explanation for this trend has been identified thus far, why 200 kW results in higher conversion
- We expect larger fire should mean larger conversion
- Validated the input files, not sure what to look at to uncover the driving factor in the trends

Additional runs are being explored at 150 and 250 kW to capture the trend



Fire Power Effect

Plots on right show isotope trend

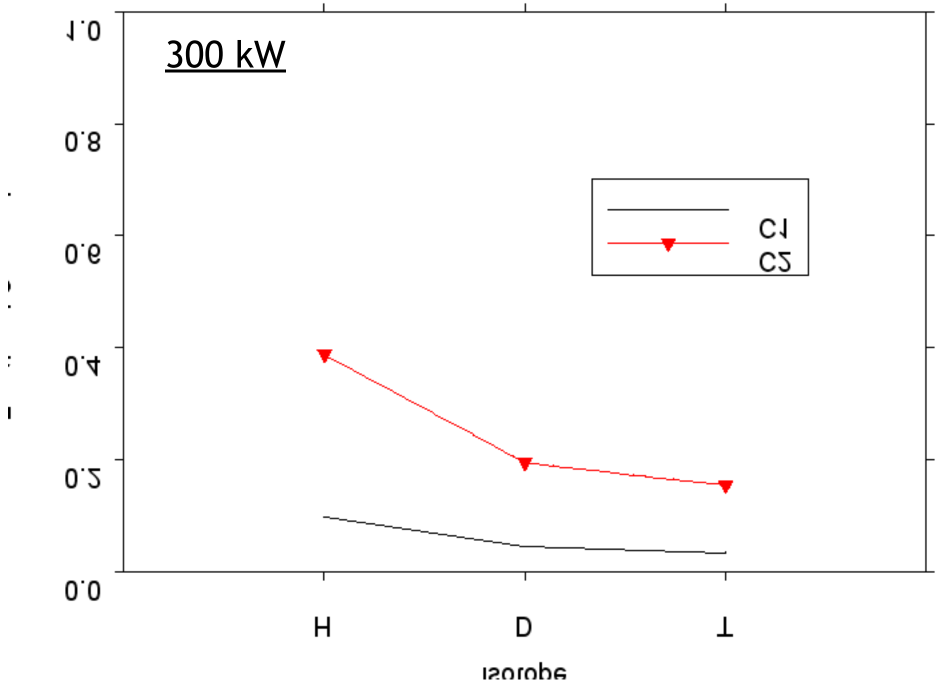
- H_2 might not be a great surrogate for T_2
- D_2 exhibits much closer behavior

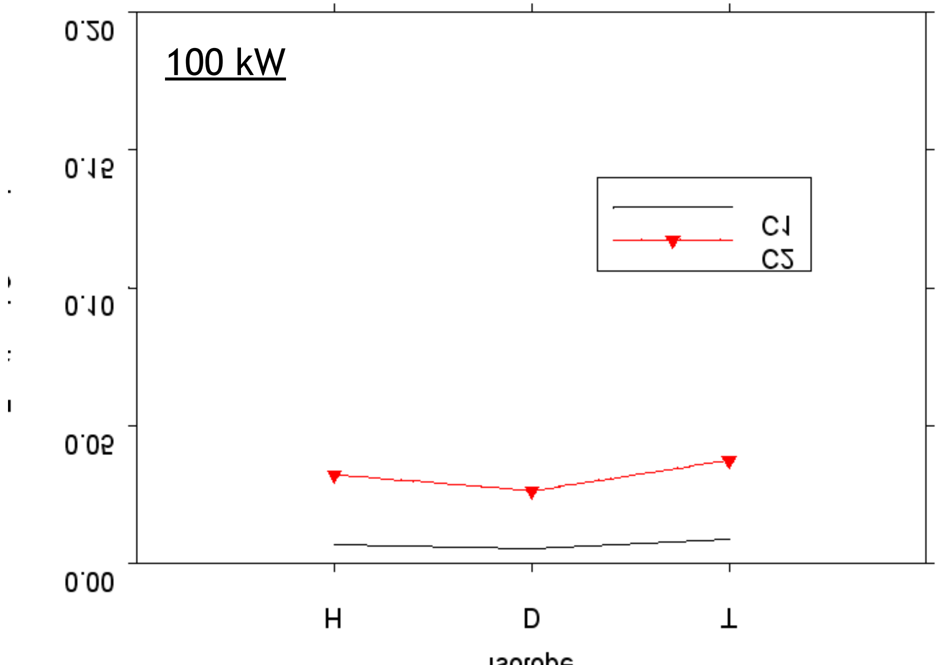
300 kW trends are clear, conversion dropping with heavier molecule

- Note the scale difference on the vertical axis

100 kW trends flat, not as apparent

- Conversion is very low all-around





Isotope 300 kW Centroids

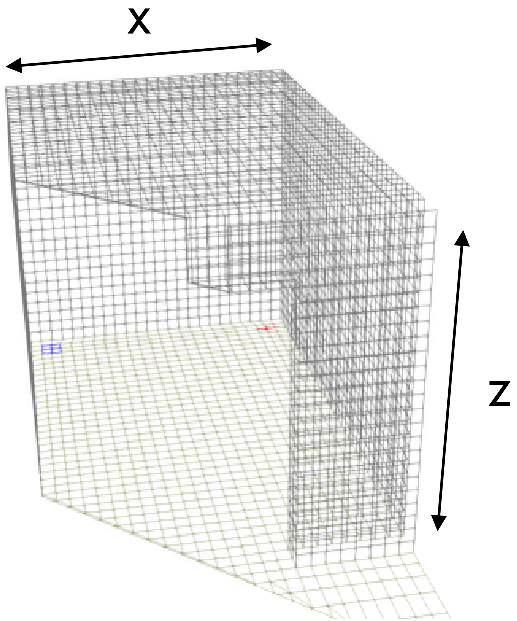
These plots on the right show centroid of ^nH concentration versus time for the 300 kW scenarios

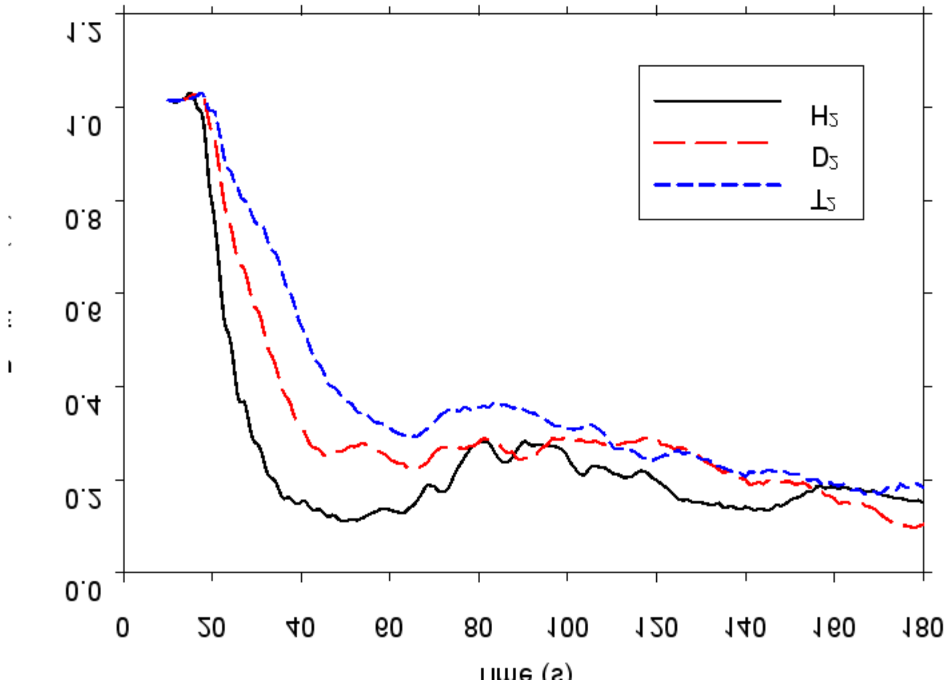
- Protium migrates fastest from initial centroidal position

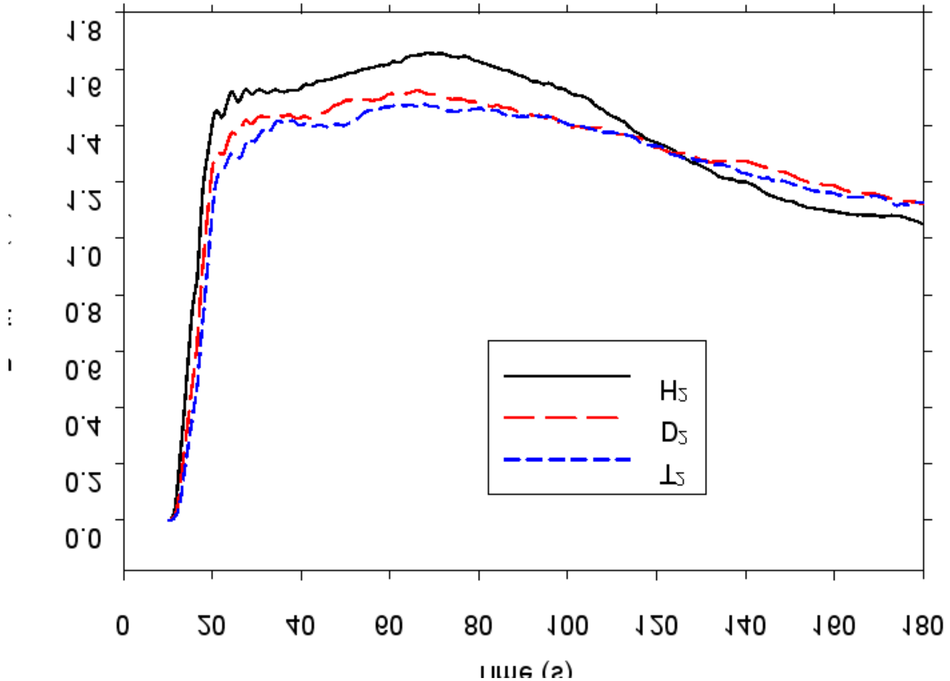
Lateral (x) spread faster for H_2-faster diffusion and advection

Vertical H_2 spread (z) faster, driven by buoyancy in addition to diffusion

- The fire is nearly identical for each isotope, so the persistently higher H_2 centroid is suggestive of a buoyancy effect







Future Work

Fill out gaps in the present simulation matrix

- Intermediate fire power conditions (150 and 250 kW)
- Move the release radially around the fire at baseline (100%) distance
- Finish fine simulation

Testing

- We are actively reacting trace H_2 and D_2 in air to deduce a relevant global reaction rate for non-flaming reaction of isotopes
  - We still won't have a rate for T_2, but we should have good trending information
- Considering other ways to validate models

Simulations

- Leverage existing model to explore other conditions

Summary

Introduced three main problems associated with computational tritium fire safety

- Problem #1 is that there are few sources for physical properties and fire performance for tritium
  - Randy Shurtz' paper in this same conference addresses this
- Problem #2 is that computational tools require verification and validation for credibility
  - Historical V&V helps with this
  - In progress tests with ^{1}H and ^{2}H also are expected to contribute to the credibility through comparisons
- Problem #3 is that there are a near infinite combination of scenarios of potential interest
  - This effort seeks to introduce a standard fire that may help key in on realistic performance behaviors

Simulations of small releases of T_2 show a low conversion fraction, with proximity to the fire being a major factor affecting conversion to T_2O

- 100 kW scenarios (per the standard) resulted in very low conversion
- Size of fire also a major factor; uncertain parameters (kinetic rate and diffusion) not showing significant effects

The buoyancy/diffusion effect appears to dominate consequence for these releases, meaning H_2 is not a particularly good surrogate, D_2 is clearly better

Model validation work in progress……

Extras