PURDUE CAPSTONE PROJECT 3M

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Contents

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I. INTRODUCTION

INTRODUCTION

Objective

Identify consequences related to hazardous chemicals;

Build models to prevent and mitigate severity of accidents.

Chemicals

Toluene; MEK(Methyl Ethyl Ketone); IPA(Isopropanol); Ethyl Acetate

Software

FDS-SMV(Fire Dynamics Simulation-Smokeview); CFD; Microsoft Excel

Reference

API 752(American Petroleum Institute); Guidelines from CCPS(Center for Chemical Process Safety); FDS-SMV User's Guide etc.

II. INDOOR MODELING

CORE PARAMETERS

FACTORS AFFECTING SEVERITY OF	Mass of fuel released	Flame speed	Energy released	Overpressure	Reflection parameters	Ventilation	Fill level	Failure pressure	Fluid temperature	Fragment projectiles
Vapor Cloud Explosion	✓	✓	✓	✓	✓	✓	×	×	×	×
Pressure Vessel Burst	×	×	✓	✓	✓	×	✓	✓	✓	✓
Fire	✓	×	×	×	×	✓	×	×	✓	×
Toxic Release	✓	×	×	×	×	×	×	×	✓	×

FACTORS AFFECTING SEVERITY OF	Composition	Operating pressure	Event duration	Thermal flux	Flammable gas concentration	Release rate	Endpoint of analysis	Toxic concentration and time	Occupant vulnerability
Vapor Cloud Explosion	×	×	×	×	×	×	×	×	×
Pressure Vessel Burst	×	×	×	×	×	×	×	×	×
Fire	✓	✓	✓	✓	✓	✓	×	×	×
Toxic Release	✓	✓	✓	×	×	×	✓	✓	✓

- Mass of Fuel released
- Overpressure
- Ventilation
- Fluid Temperature
- Event Duration
- Thermal Flux
- Flammable Gas Concentration
- Release Rate
- Toxic Concentration and Time

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TNT MODEL

TOLUENE	
Heat of Combustion (MJ/kg)	42.54
Specific heat (kJ/kg/K)	2.02
Latent heat (kJ/kg)	351
Boiling temperature (K)	383.8
Ambient temperature (K)	293
Heat of Combustion TNT (MJ/kg)	4.68
Mass of fuel released (kg)	100

$$Flash\ fraction, F = 1 - exp\left[\frac{C_P \Delta T}{L}\right] = 1 - exp\left[\frac{2.02\,\frac{\text{kJ}}{\text{kg.K}} \times (298.15 - 383.8)}{351}\right] = 0.41$$

$$Weight\ of\ fuel\ released, W_f = 2 \times 0.41 \times 100 = 81.4\ \text{kg of Toluene}$$

$$TNT\ equivalent\ weight, W_{\text{TNT}} = \alpha_e \frac{W_f H_f}{H_{\text{TNT}}} = 0.03 \times \frac{81.4\ \text{kg} \times 42.54\ \text{MJ/kg}}{4.68\text{MJ/kg}} = 22.2\ \text{kg}$$

$$where, C_p = Specific\ heat\ \left(\frac{kJ}{kg.K}\right); L = Latent\ heat\ \left(\frac{kJ}{kg}\right); \alpha_e = Efficiency\ factor$$

$$H_{TNT} = TNT\ heat\ of\ detonation\ \left(\frac{MJ}{kg}\right);\ H_f = Heat\ of\ combustion\ \left(\frac{MJ}{kg}\right)$$

$$Scaled\ distance, R' = \frac{R}{W_{TNT}^{1/3}}\ ; where, R = actual\ distance\ from\ explosion$$

Distance from charge (m)	Distance from charge (ft)	Scaled distance from charge (m/kg$^{1/3}$)	Side-on peak overpressure (kPa)
3	10	1.07	1215.9
6	20	2.13	253.3
8	26	2.85	101.3
15	49	5.34	40.5
30	98	10.67	15.2
60	197	21.35	5.1

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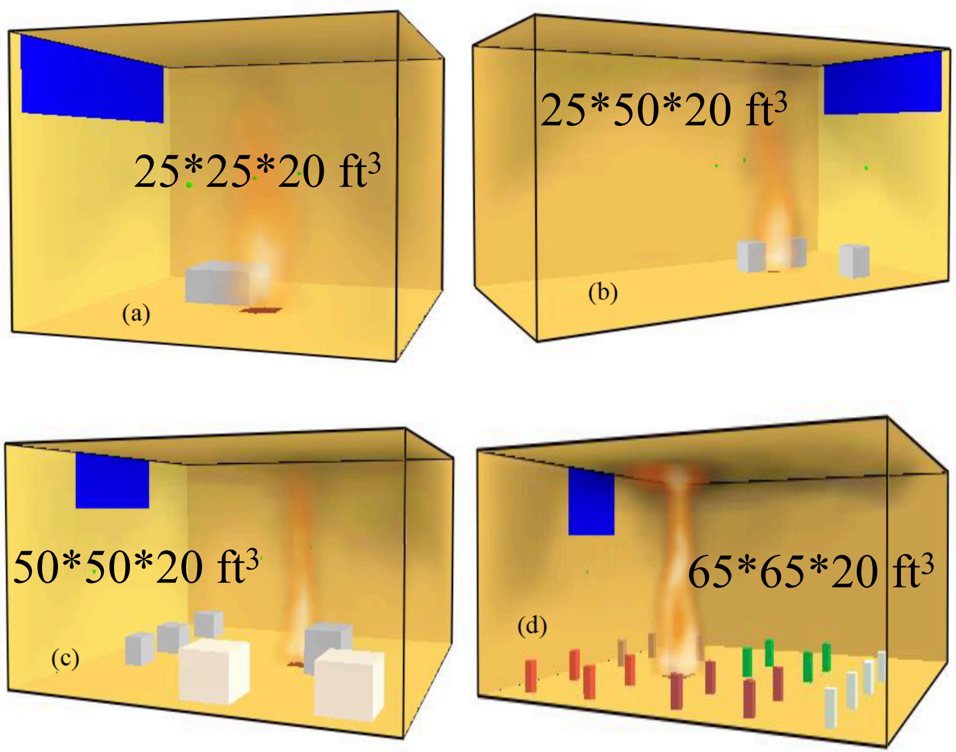
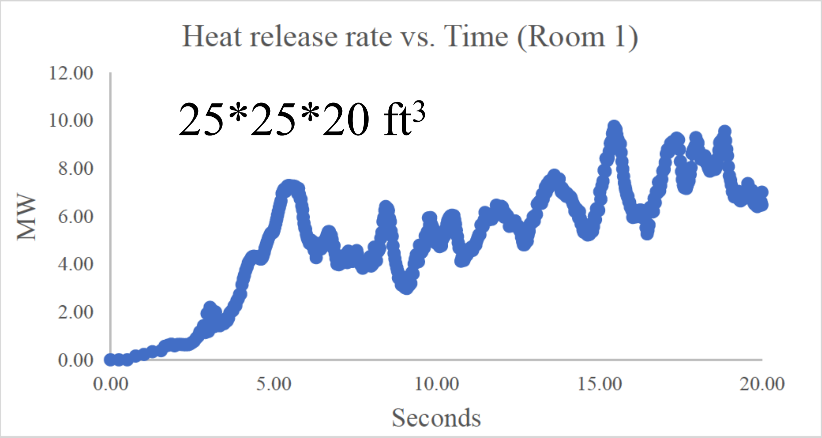
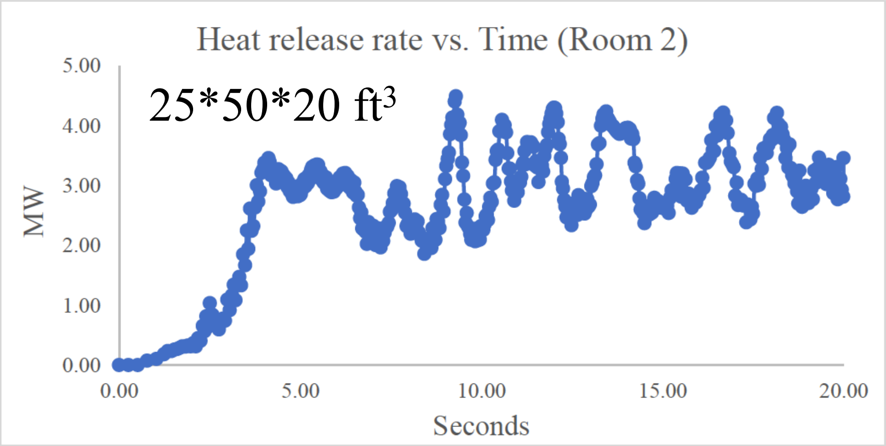
FIRE SIMULATIONS BY FDS

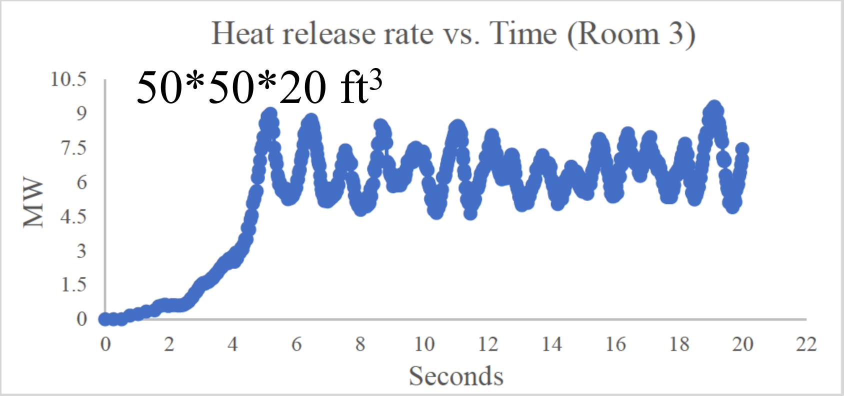


- Temperature Range: 20˚C to 1200 ˚C
- Lethal Temperature: 5 sec to 12 sec

FIRE SIMULATIONS BY FDS

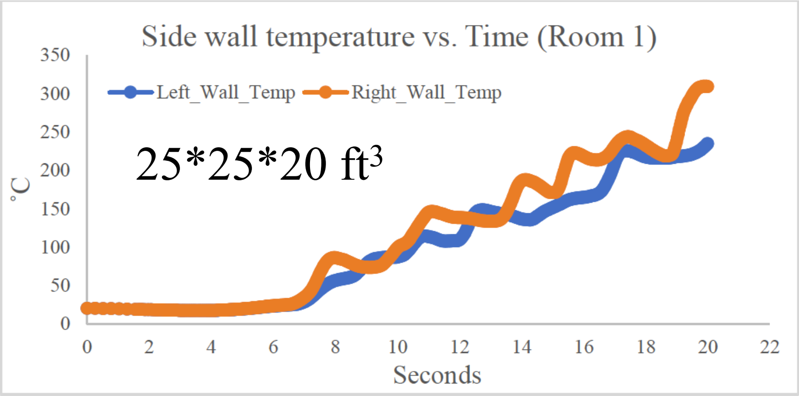


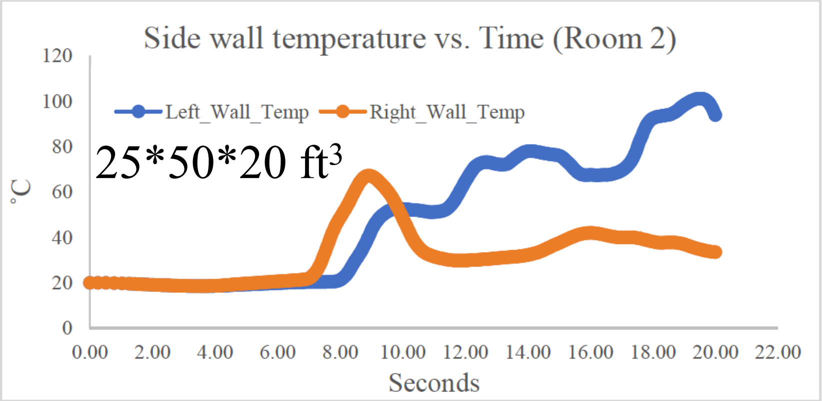


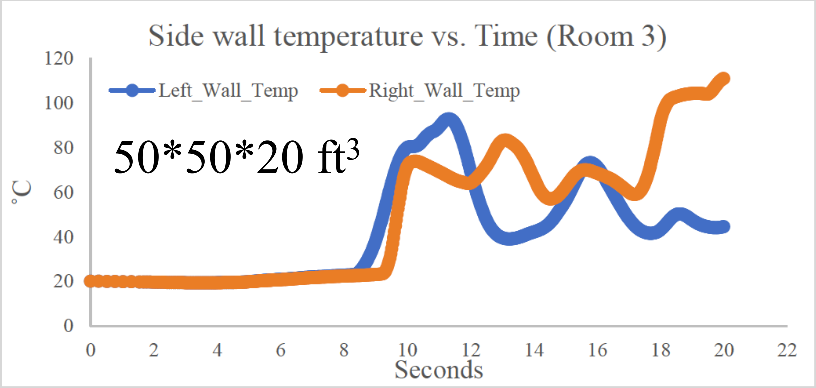


- Heat Release Rate (General):
  Room3 > Room1 > Room2
- Within a certain range of room size, heat release rate increases as the size decreases.
- Out of the range of room size, longer fire duration and higher heat release rate may occur due to more oxygen in the room.

FIRE SIMULATIONS BY FDS

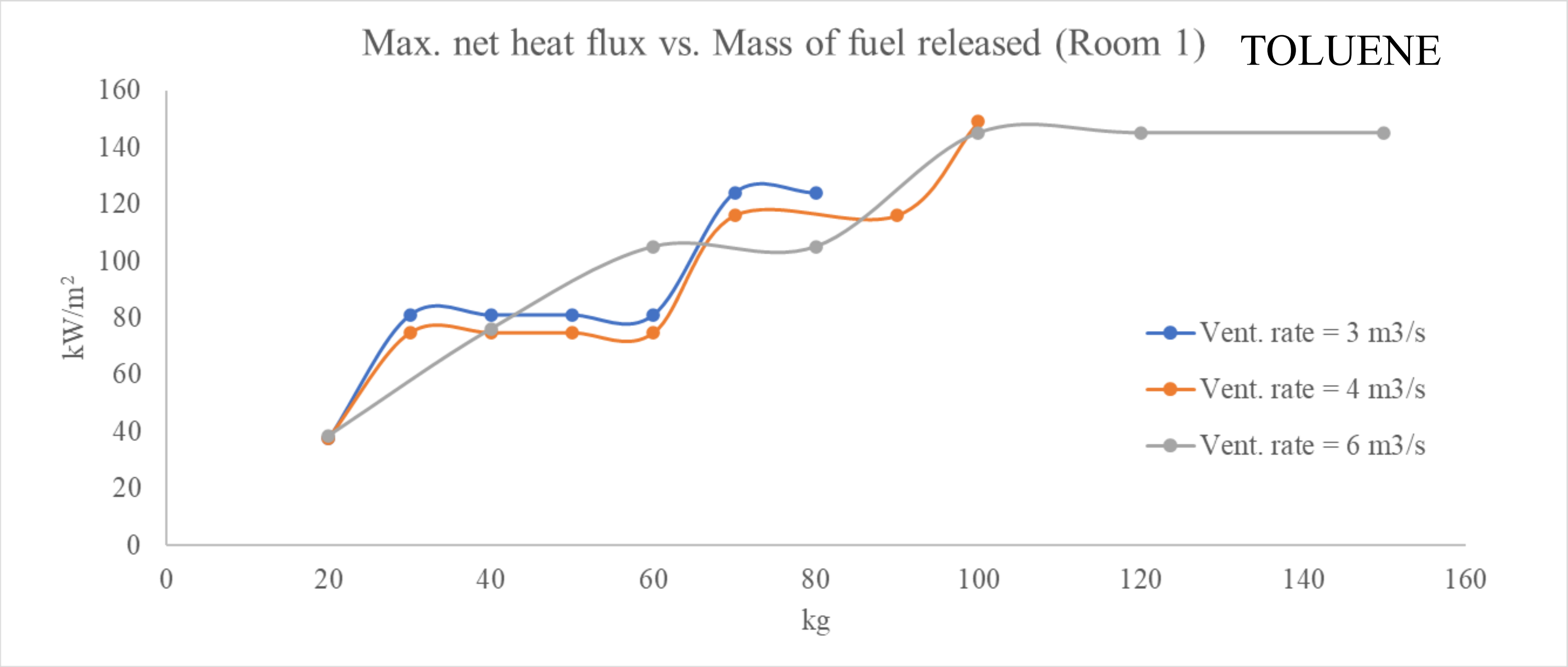






- Max. Side Wall Temperature:
  Room3 > Room1 > Room2
- Within a certain range of room size, side wall temperature increases as the size decreases.
- Out of the range of room size, higher side wall temperature may occur due to longer fire duration.

EFFECT OF VENTILATION



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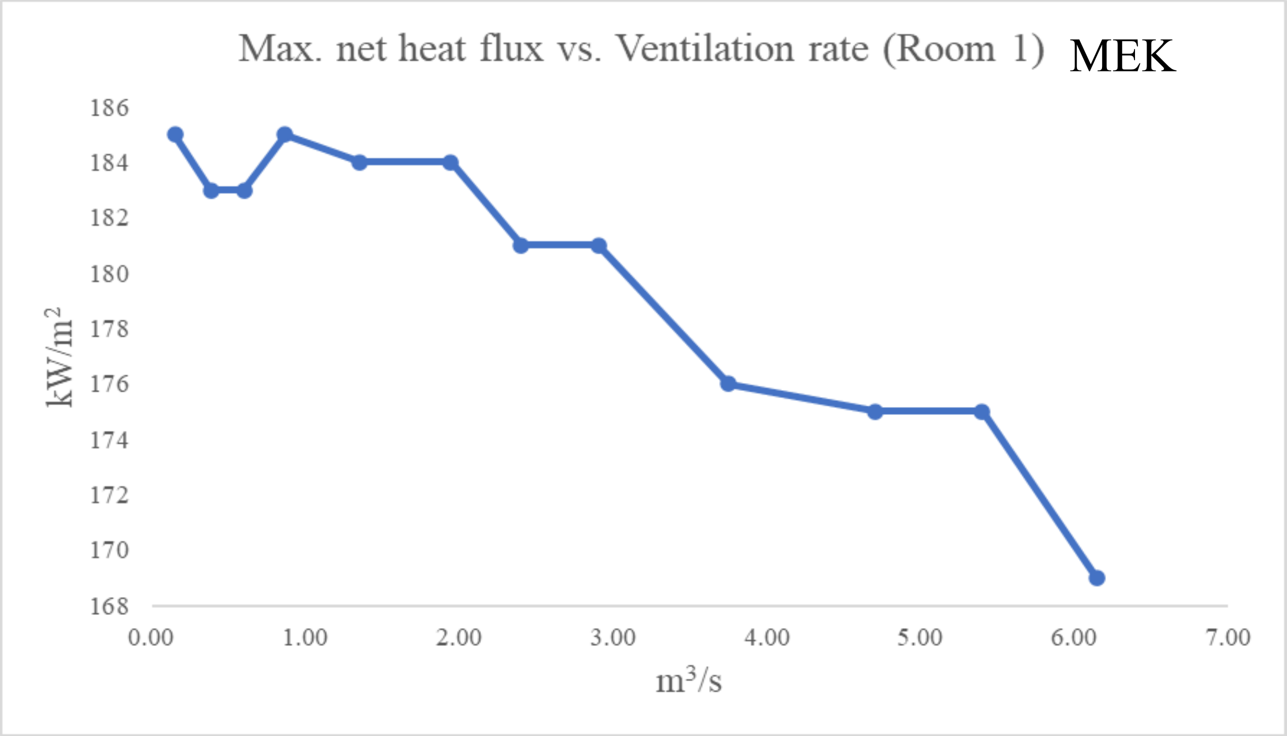
EFFECT OF VENTILATION



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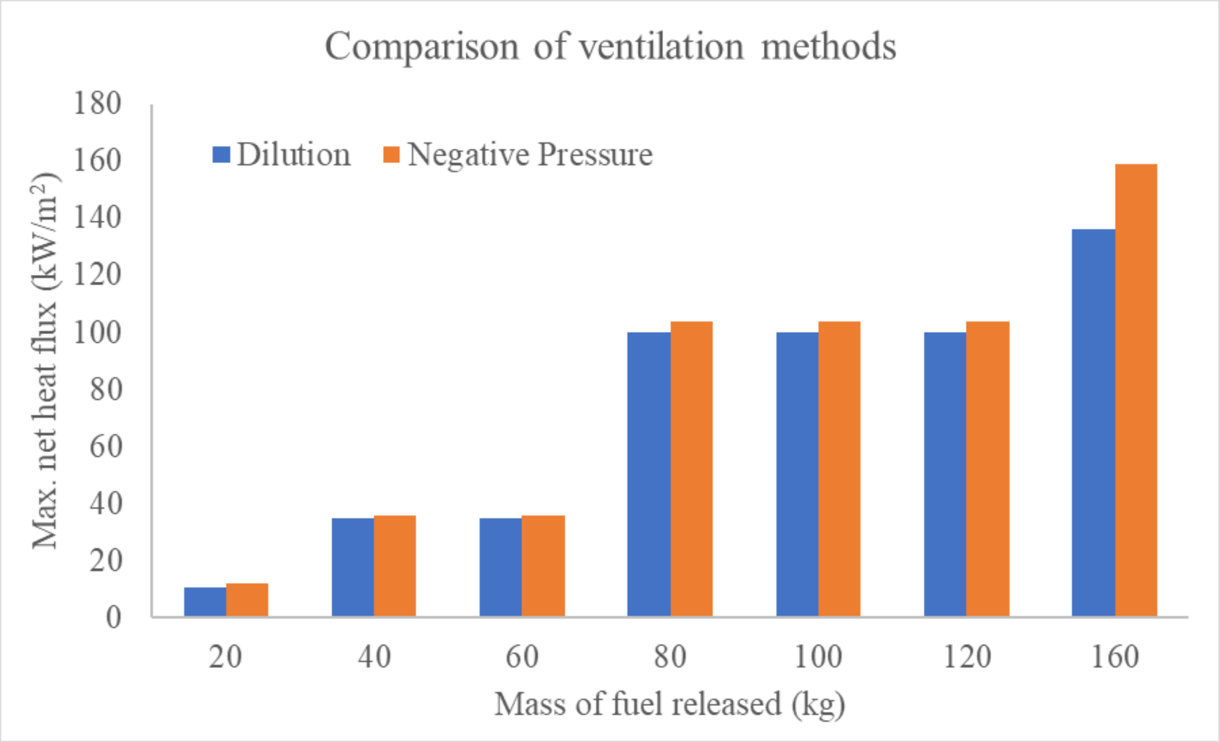
EFFECT OF VENTILATION



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EXPLOSION AND TOXIC RELEASE MODEL

TOLUENE		
Mass of Fuel released	M (kg)	39.80
Ambient Temperature	T (K)	298
Non-ideal Mixing Factor	k	0.1
Area of Ventilation	A_v (m^2)	10
Control velocity	u (m/s)	0.6
Liquid Pool Thickness	(m)	0.05
Absolute Pressure	P (atm)	1
Liquid Temperature	T_L (K)	298
Evaporation Rate	Q_m (g/min)	37.35
Mass Transfer Coeff. For Area A	K (m/s)	0.0048
Area of Pool	A (m^2)	0.92
Saturation Vapor Pressure	P^{sat} (atm)	0.037
Gas constant	R_g (m^3 atm mol^{-1} K^{-1})	0.00008205
Molecular Weight	MW	92.14
Density	kg/m^3	862
Ventilation Rate	Q_v (m^3/s)	6
STEL	(ppm)	150
Lower Explosive Limit	LEL (ppm)	1100
Upper Explosive Limit	UEL (ppm)	7100
25% LEL	(ppm)	275
Permissible Exposure Limit	PEL (ppm)	200
TLV-TWA	(ppm)	20
IDLH	(ppm)	500
Concentration	C (ppm)	275.33

INSTRUCTIONS

Only parameters that can be changed are:
Mass of Fuel released
Ambient Temperature
Non-ideal Mixing Factor
Area of Ventilation
Control velocity
Liquid Pool Thickness
Absolute Pressure
Liquid Temperature

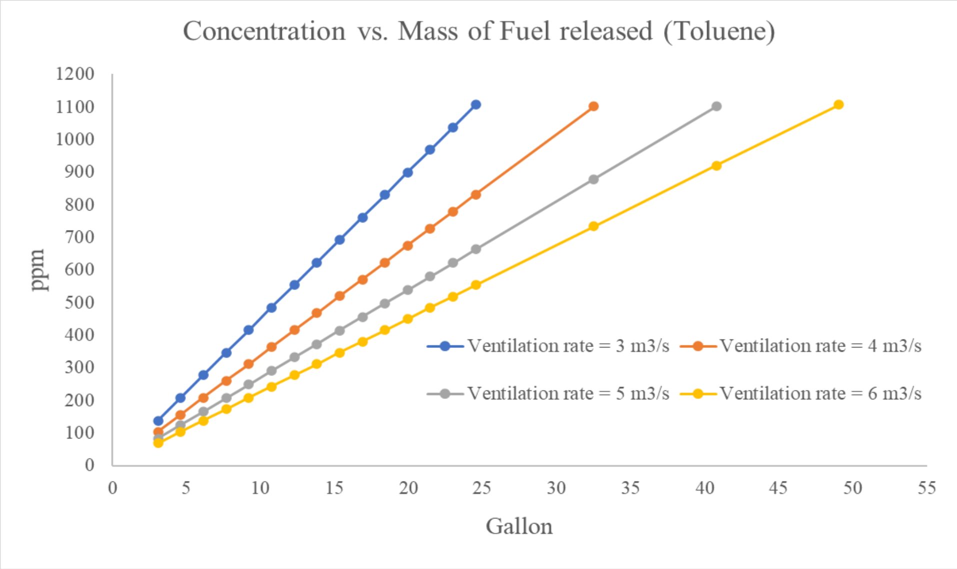
1) Enter value of *Mass of Fuel released* in kg and *Ambient Temperature* in K.
2) Enter value of *Non-ideal Mixing Factor*. The value ranges from 0.1-0.5. Use 0.1 for worst case scenario and 0.125 for average mixing.
3) Enter *Area of Ventilation* in m^2, according to the vent size (*length x width*).
4) Enter value of *Control velocity* in m/s. Generally used values are in the range 0.4-0.6 m/s.
5) Enter value of *Liquid Pool Thickness* in m.
6) Enter *Liquid Temperature* in K and *Absolute Pressure* in atm.
6) See calculated value of *Concentration*, to compare with explosive limits and occupational exposure limits.
7) Value of *Concentration* in red indicates presence of explosive concentration.

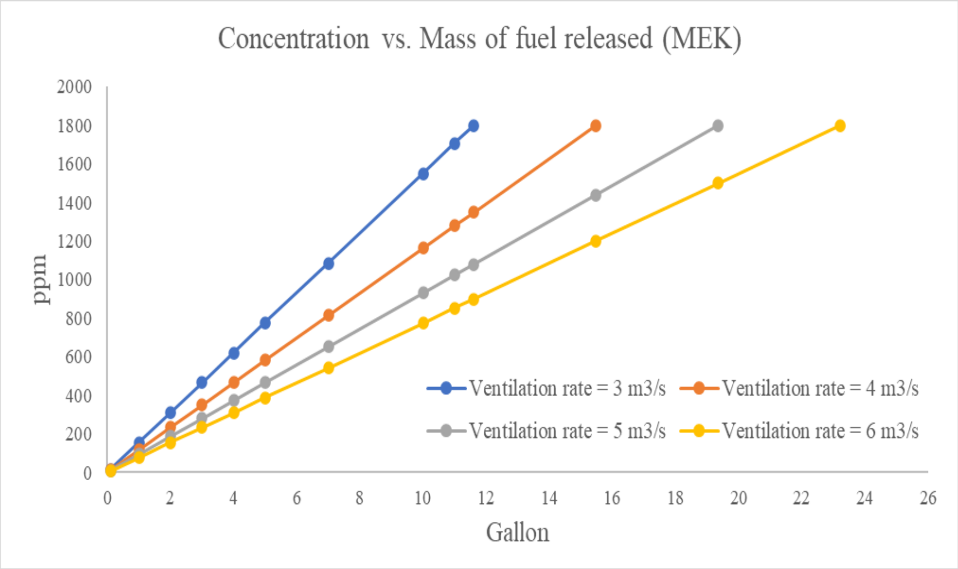
EXPLOSION AND TOXIC RELEASE MODEL

- Quantity of spill resulting in 25% LEL concentration

Chemical	Mass of fuel released (gallons)			
	Ventilation rate = 3 m^3/s	Ventilation rate = 4 m^3/s	Ventilation rate = 5 m^3/s	Ventilation rate = 6 m^3/s
Toluene	6.1	8.1	10.1	12.2
MEK	2.9	3.86	4.83	5.8
Isopropanol	6.4	8.5	10.6	12.8
Ethyl Acetate	3.6	4.8	6.03	7.2

CONCENTRATION VS. MASS OF FUEL RELEASED





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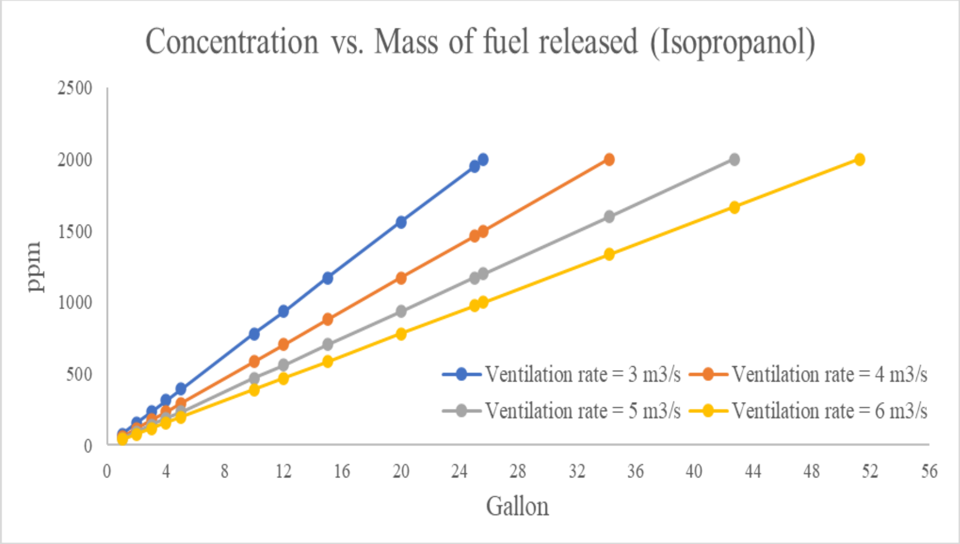
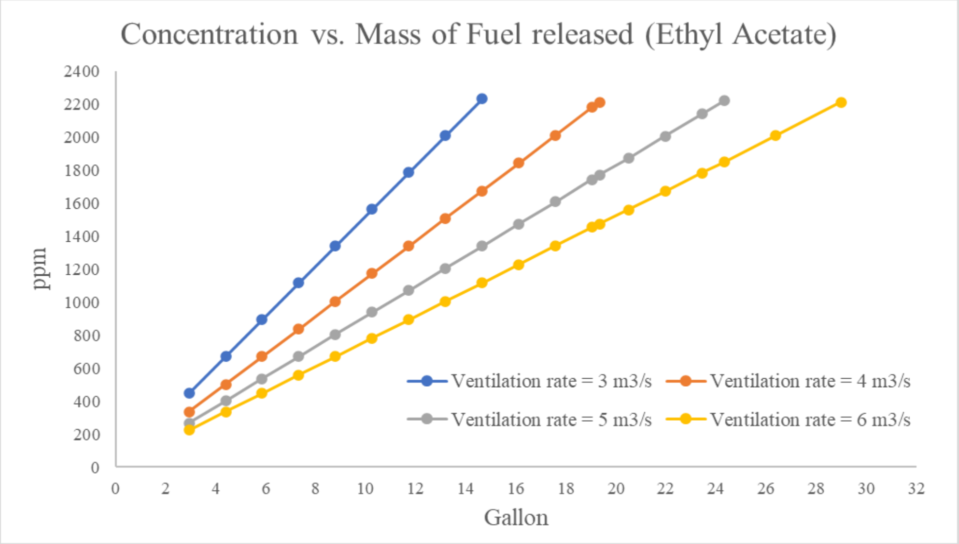
CONCENTRATION VS. MASS OF FUEL RELEASED





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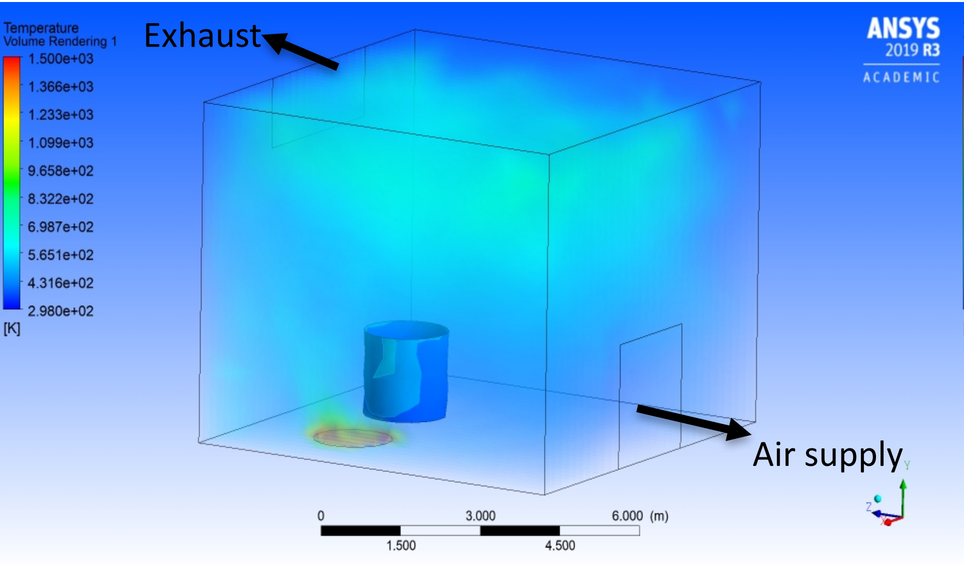
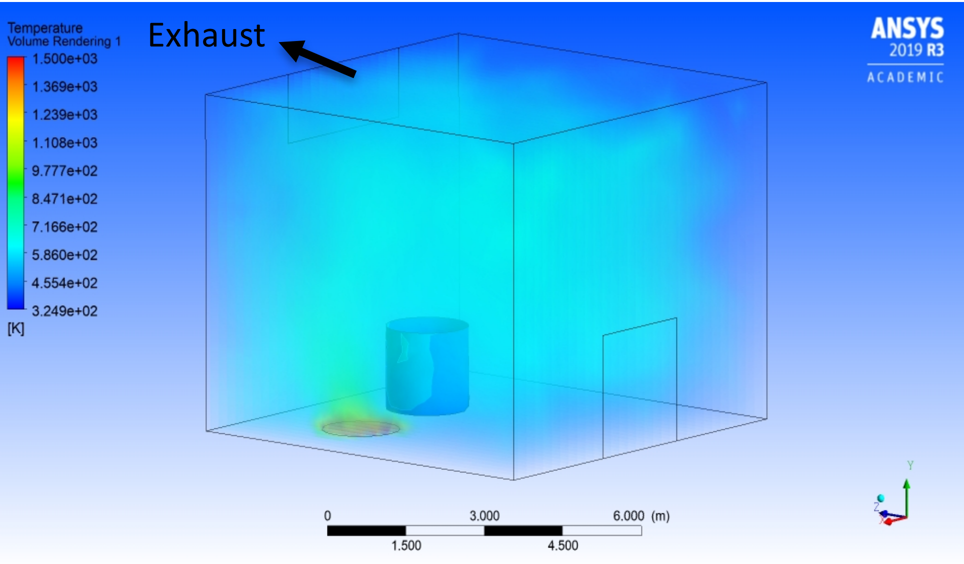
CFD MODEL FOR FIRE



Dilution ventilation



Negative pressure ventilation

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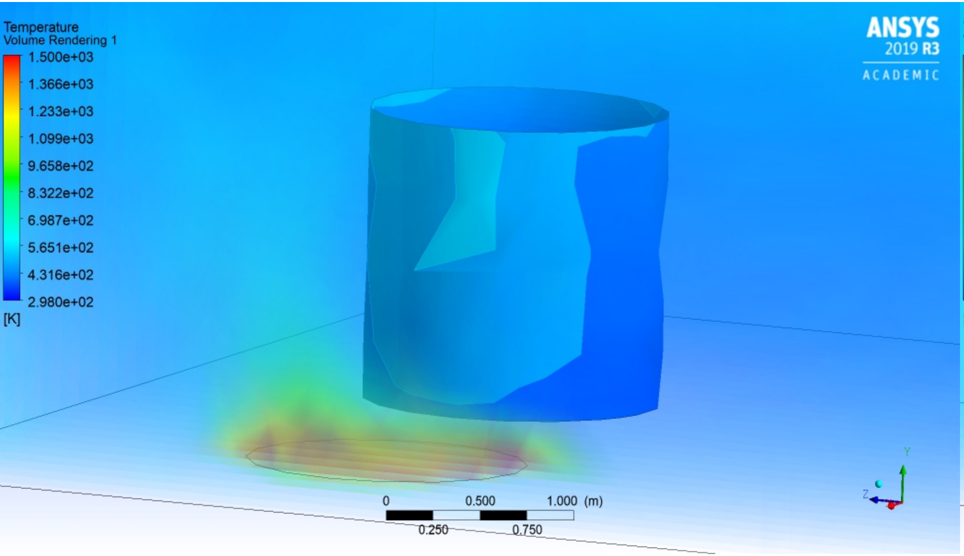
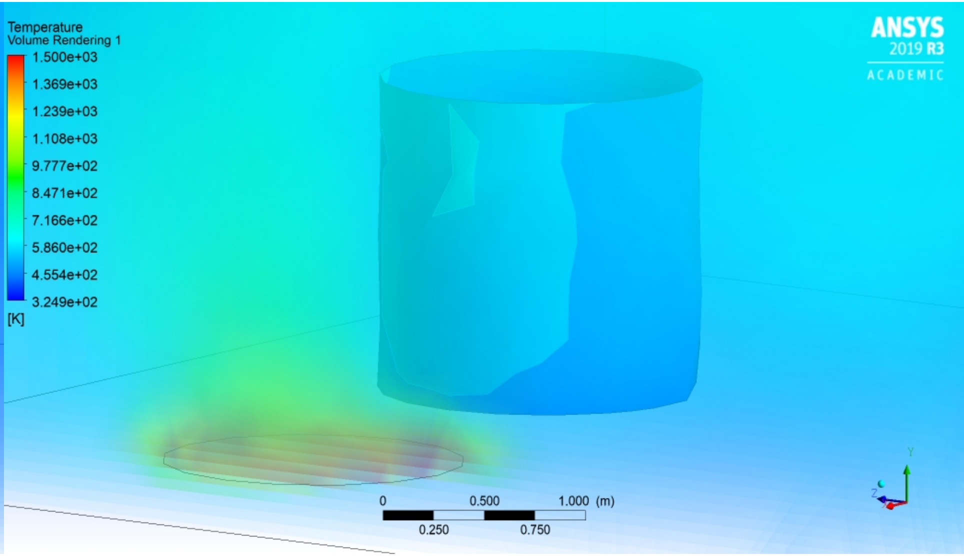
CFD MODEL FOR FIRE



Dilution ventilation



Negative pressure ventilation

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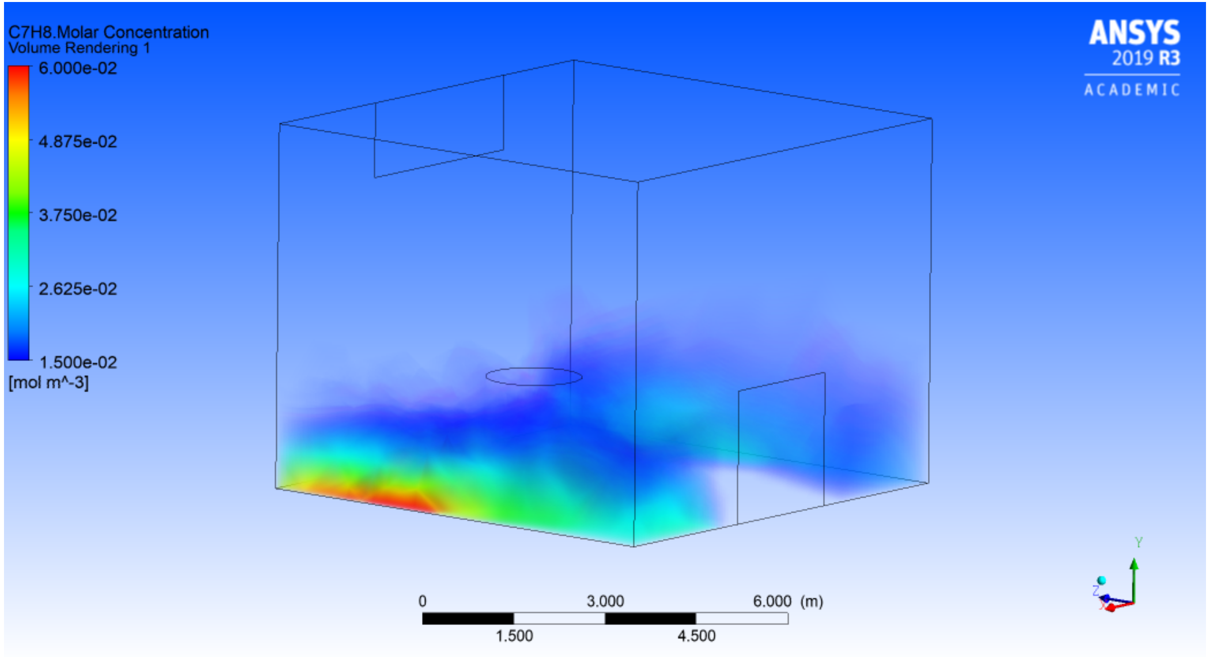
CFD MODEL FOR TOXIC RELEASE



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SUMMARY

Literature review → Identification of core parameters → Fire models → Control methods → Explosion and toxic release model → CFD models

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CONCLUSION

- Consequence-based assessment is essential to understand potential accidents and to identify its severity.
- Adequate control measures can be installed.
- Quantitative risk assessments are crucial.
- Inherently safer designs can reduce chance of accidents.
- Follow Recognized and Generally Accepted Good Engineering Practices (RAGAGEP)
- Prevention is always better than mitigation.

THANK YOU

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