Fire Plume Modeling

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Industrial Plumes vs. Large Fires



Gaussian Models

Fire Models

Talk Outline

- Part 1: Background
 - Fires: Photos & Diagrams
 - Fire Modeling: Basic Inputs & Parameters
 - Modeling Goals and Strategies
- Part 2: CFD Modeling of Fires using FDS
 - Model Description, Setup, I/O
 - Pool Fire Test Case (Neutral Atmospheric Stability)
 - Pool Fire Test Case (Stable Atmospheric Stability)
- Part 3: Modeling with BUOYANT
 - Non-CFD: Steady-State Plume Model with fire plume rise model
 - Test Cases: How much of fire plume resides in ABL?

Part 1: Background

Large Industrial Fires





- Heat and Mass Fluxes
- Buoyancy Flux = Heat Release Rate x Area of Release
- Plume Rise, Plume Buoyancy, Clean Air Entrainment
- Constituents: Carbon Dioxide, Smoke, Trace Metals, others

Large Industrial Fires



- Plume Rise through the Atmospheric Boundary Layer?
- Penetration into the inversion capping the ABL

Fire Dispersion: Physics & Modeling (1)



Kukkonen et al (2022); <u>https://gmd.copernicus.org/articles/15/4027/2022/</u>

Fire Dispersion Physics & Modeling (2)

Top of the boundary layer



Kukkonen et al (2000); https://link.springer.com/chapter/10.1007/978-1-4615-4153-0_55

Fire Modeling: Basic Inputs & Parameters (Emissions)

Heat & Mass Release Rate

 $qHc = \Delta Hc x mfuel$

where:

qHc = the heat release rate (kJ/s = kW)

 Δ Hc = the heat of combustion (MJ/kg)

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mfuel = the mass flow rate of the fuel (g/s)
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Fire Modeling: Basic Inputs & Parameters (Emissions)

Example: Pool Fires

Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0Heptane (C_7H_{16}) 44 6000.1011.12.850.010.0040.0Kerosene43 2000.0393.52.830.0120.0040.0LNG (mostly CH_4)50 0000.0781.12.72LPG (mostly C_3H_8)46 0000.0991.42.850.0050.0010.0	Heat of Combustion		Mass Release Rate (Infinite-diameter pool)			Yields		
Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0Heptane (C_7H_{16}) 44 6000.1011.12.850.010.0040.0Kerosene43 2000.0393.52.830.0120.0040.0LNG (mostly CH_4)50 0000.0781.12.72LPG (mostly C_3H_8)46 0000.0991.42.850.0050.0010.0						γ		
Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0Heptane (C_7H_{16}) 44 6000.1011.12.850.010.0040.0Kerosene43 2000.0393.52.830.0120.0040.0LNG (mostly CH_4)50 0000.0781.12.72	LPG (mostly C ₃ H ₈)	46 000	0.099	1.4	2.85	0.005	0.001	0.024
Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0Heptane (C_7H_{16}) 44 6000.1011.12.850.010.0040.0Kerosene43 2000.0393.52.830.0120.0040.0	LNG (mostly CH ₄)	50 000	0.078	1.1	2.72	_	_	_
Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0Heptane (C_7H_{16}) 44 6000.1011.12.850.010.0040.0	Kerosene	43 200	0.039	3.5	2.83	0.012	0.004	0.042
Acetone (C_3H_6O) 25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6) 40 1000.0852.72.330.0670.0180.1Butane (C_4H_{10}) 45 7000.0782.72.850.0070.0030.0	Heptane (C ₇ H ₁₆)	44 600	0.101	1.1	2.85	0.01	0.004	0.037
Acetone (C_3H_6O)25 8000.0411.92.140.0030.0010.0Benzene (C_6H_6)40 1000.0852.72.330.0670.0180.1	Butane (C ₄ H ₁₀)	45 700	0.078	2.7	2.85	0.007	0.003	0.029
Acetone (C ₃ H ₆ O) 25 800 0.041 1.9 2.14 0.003 0.001 0.0	Benzene (C ₆ H ₆)	40 100	0.085	2.7	2.33	0.067	0.018	0.181
	Acetone (C_3H_6O)	25 800	0.041	1.9	2.14	0.003	0.001	0.014
$kJ kg^{-1} kg (m^2 s)^{-1} m^{-1} gg^{-1} gg^{-1} gg^{-1} gg^{-1} gg^{-1}$		kJ kg ⁻¹	$kg (m^2 s)^{-1}$	m^{-1}	gg ⁻¹	gg^{-1}	gg^{-1}	gg^{-1}

Kukkonen et al (2022); <u>https://gmd.copernicus.org/articles/15/4027/2022/</u>

Fire Modeling: Basic Inputs & Parameters (Meteorological)

Dispersion

- Wind Speed
- Atmospheric Stability
- Boundary Layer Depth, Height of Inversion Base
- Atmospheric Lapse Rate above Boundary Layer

Particle Formation, Chemistry, Deposition

- Humidity
- Precipitation

Desired Features in Fire Dispersion Model

- Simple but effective inputs to characterize source characteristics
 - Mass and heat release
 - Constituents
- Proper handling of plume rise
 - Enhanced buoyancy
 - Entrainment of ambient air into rising fire plume
 - > CFD directly simulates, plume models must parameterize
- Capturing induced circulations
 - Fire-driven circulations due to strong buoyant convection
 - Need CFD for this

Fire Dispersion Models: Options

• Computational Fluid Dynamics (CFD)

- Fire Dynamics Simulator (FDS, <u>https://www.nist.gov/services-resources/software/fds-and-smokeview</u>
- Full 3-D solutions for Navier-Stokes equations
- Full suite of embedded models for fire physical processes (pyrolysis, combustion, phase change, chemistry, etc ...)
- Near-Field (within 1-km from source)

• Gaussian Dispersion Models designed for fires

- BUOYANT (<u>https://gmd.copernicus.org/articles/15/4027/2022/</u>)
- Steady-state w/ Embedded fire plume rise model
- > Far-Field (beyond 1-km from source)

Highlight: Near vs. Far-Field Modeling



Far Field, Gaussian Fire

Part 2: CFD Modeling using FDS (near-field dispersion)

Fire Dynamics Simulator (FDS): Basics

- U.S. National Institute of Standards and Technology (NIST)
- <u>https://www.nist.gov/services-resources/software/fds-and-smokeview</u>
- Computational Fluids Dynamics (CFD)
- Full Physics: Various physical processes, sub-models and configurations
- Indoor and outdoor capabilities
- Simulates fire generation/spread and dispersion of reactants/smoke
- Rectangular grid (relatively simple mesh generation ...)

Fire Dynamics Simulator (FDS) Installation & Execution

- Windows executable (no compilation necessary)
- Command line interface (no GUI)
- Enter inputs into text file
- Smokeview graphics to view output

FDS Test Runs: Grid & Fire Inputs

• Grid

- 25 x 25 x 25 m resolution over 2000 x 1000 x 1000 m domain (80 x 40 x 40)
- Surface "pool" fire of 150 x 150 m centered at (x, y, z) = (1000,500,25)

• Fire Inputs

- Single-step mixing controlled combustion
- Fuel is propane
- Heat Release Rate = 250 kW/m2
- Corresponds to a fuel consumption rate of about 0.005 kg/m2/s
- Set 10% of reactants to be smoke (by mass)

FDS Test Runs: Meteorological Inputs

- Wind: Boundary layer background flow of about 2 m/s
- Neutral Case: Set lapse rate to adiabatic (stability class D)
- Stable Case: Set lapse rate to isothermal (stability class E or F)

Compare output for neutral vs. stable

FDS Test Runs: Procedure

- 14400 seconds integration time (= 4 hours)
- "Turn on" fire @ t = 7200
 - 0 < t < 7200: "spin up" period to bring background wind to quasi steady-state
 7200 < t < 14400: "fire period"
- After period of build-up of fire @ t = 7200, new "fire-affected" quasi steady-state is reached by around t = 8400.
- Plots to be shown are @ t = 14400 (final time)

Neutral: Smoke & Temperature (image)



Neutral: Smoke and Temperature (video link)





Neutral: Smoke & Winds (image)

0.0

Stable: Smoke & Temperature (image)



Stable: Smoke and Temperature (video link)	─ Slice temp C
	51.77
	48.26
	44.75
	41.24
	37.73
	34.22
	30.71
	27.2
	23.69
	20.18
	16.67

Stable: Smoke & Winds (image)



Smoke visuals @ t = 2 hours after fire start

z = 1000 m



Neutral

Stable

Smoke visuals overlaid w temperature (deg C) @ t = 2 hours after fire start



Flow vectors @ t = 2 hours after fire start

Stable



Stable

Neutral

PM2.5 (ug/m3) vs. Height (meters) @ different downwind distances from fire



Ground Level PM2.5 Concentrations (ug/m3) vs. Downwind Distance from Fire (m)



PM2.5 (ug/m3)

Part 3: Gaussian Plume Modeling using BUOYANT

Reminder: Near vs. Far-Field Modeling



BUOYANT: Basics

- Finnish Meteorological Institute
- <u>https://gmd.copernicus.org/articles/15/4027/2022/</u>
- Steady-State Gaussian plume model
- Embedded fire plume rise model
- Far-field dispersion (> 1 km)

BUOYANT: Installation & Execution

- FORTRAN code (compilation necessary)
- Need to install FORTRAN compiler
- MSYS2 virtual LINUX required on WINDOWS, has 'gfortran' as a package
- Command line interface (no GUI)
- Enter inputs into text file
- Text file outputs

Large Industrial Fires



- Question ... how much of the plume stays within the ABL?
- Run cases to check how model predicts this quantity.

BUOYANT: Test Runs

Meteorological Inputs

- Wind Speed = 3.22 m/s
- Neutral ABL w depth = 1000 m
- Pool Fire: Case 1 ("low' heat release)
 - Heat Release Rate = 20 kW/m2
- Pool Fire: Case 2 ("medium" heat release)
 - Heat Release Rate = 700 kW/m2
- Pool Fire: Case 3 ("high" heat release)
 - Heat Release Rate = 1800 kW/m2

Reminder: FDS Test Runs

• Grid

- 25 x 25 x 25 m resolution over 2000 x 1000 x 1000 m domain (80 x 40 x 40)
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• Fire Inputs

- Single-step mixing controlled combustion
- Fuel is propane
- Heat Release Rate = 250 kW/m2
- Corresponds to a fuel consumption rate of about 0.005 kg/m2/s
- Set 10% of reactants to be smoke (by mass)

BUOYANT Test Runs: Results

(Fraction of plume that stays in the ABL)

Modeling Run	Heat Release Rate (kW/m2)	Fraction of Plume in ABL
Case 1 (Low Heat Release)	20	0.5597
Case 2 (Medium Heat Release)	700	0.1874
Case 3 (High Heat Release)	1800	0.05533

- Fraction in ABL highly sensitive to fire strength (via heat release)
- More plume in ABL \rightarrow High surface concentration
- Appears to capture an observable feature of strong fires ... that most plume mass can stay aloft above ABL

Conclusions

Dispersion Modeling for Fires

- Two approaches demonstrated as alternatives to typical Gaussian models
- Initial test results of both appear promising
- Computational Fluid Dynamics, CFD)
 Fire Dynamics Simulator (FDS)

2. Steady-Steady Gaussian Modeling with Fire Plume Rise **BUOYANT**