A. TROUVÉ

Codes Incendies

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CFD-Based Compartment Fire Modeling

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CFD-Based Compartment Fire Modeling

• Outline
  ➢ Overview of Compartment Fire Dynamics
  ➢ Overview of Fire Modeling
  ➢ Examples of Compartment Fire Simulations
Compartment Fires

- **Example:**
  - *Sequence of events:* localized ignition of Christmas tree; rapid fire spread (fuel sources = Christmas tree, wall lining, armchair and sofa, lamp shade, drawer chest and table, carpet, bunny toy); rapid filling of compartment with smoke; transition to flashover
  - Test conducted by the National Institute of Standards and Technology
Compartment Fires

• Example:
Compartment Fires

- **Main features**: fire is an unusual combustion process in which the fuel supply corresponds to a large list of flammable objects and materials, usually in solid or liquid form
  - solids (wood, plastics, foams, fabric, linings, *etc*)
  - liquids (engine fuels, LNG, melted solids, *etc*)
Compartment Fires

- **Main features**: fire is an unusual combustion process in which the fuel supply is unknown
  - Typical production of flammable vapors in a fire:
    - Consider a flammable solid object/material that is a potential fuel source
    - At ambient temperature, the fuel is in solid form, the oxygen (from air) in gaseous form, and there is no combustion
    - At moderately elevated temperatures (typically 200-400 degrees Celsius), a complex thermal degradation process is initiated in the solid object/material, that corresponds to a phase change and produces fuel in gaseous form. This gasification process is called pyrolysis.
Main features: fire is an unusual combustion process in which the fuel supply is unknown

- Typical production of flammable vapors in a fire:
  - The fuel gasification rate is determined by a heat feedback mechanism
    - Fuel gasification is an endothermic process and heat comes from the gas-to-solid heat transfer
    - The fuel gasification rate is controlled by the rate of gas-to-solid heat transfer
• **Main features:** fire is an unusual combustion process in which
  the fuel supply is unknown
  - Typical production of flammable vapors in a fire:
  - The gas-to-solid thermal feedback controls the fuel mass loss rate and thereby the overall fire size

  The fraction of energy fed back to the fuel source is typically a small fraction of the energy released by combustion:

  \[
  \chi_{\text{feedback}} \approx \frac{\Delta H_{\text{pyro}}}{\Delta H_{\text{comb}}} \approx 0.01 - 0.06
  \]

  - The thermal feedback has 2 components corresponding to convective and radiative heat transfer
Compartment Fires

- **Main features**: fire is a buoyancy-driven, relatively-slow, non-premixed combustion process
  - *Example*: pool fire configuration
    - Fuel source velocity is small (a few cm/s)
    - Buoyancy effects accelerate the flow up to several m/s; flow regime corresponds to moderate turbulence intensities
    - Flame corresponds to diffusion combustion and to a thin reaction sheet where fuel and air meet in stoichiometric proportions
    - Slow velocities and long residence times promote soot formation and radiant losses
      \[ \chi_{rad} = \left( \dot{Q}_{rad} / \dot{Q}_{comb} \right) \sim 35\% \]

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Main features: fire is a buoyancy-driven, relatively-slow, non-premixed combustion process

- Example: pool fire configuration
  - Flame height scales with Froude number

\[
Fr_F = \frac{u_F (Z_{st})^{3/2}}{[\left(\frac{\Delta T_f}{T_\infty}\right) g d_F \left(\frac{\rho_F}{\rho_\infty}\right)^{1/2}]^{1/2}}
\]

\[
\dot{Q}^* = \frac{\dot{Q}_{comb}}{\rho_\infty c_{p,\infty} T_\infty \sqrt{gd_F d_F}} \sim Fr_F
\]
**Compartment Fires**

- **Main features**: fire is a buoyancy-driven, relatively-slow, non-premixed combustion process
  - Example: pool fire configuration

- **Buoyancy**-driven flame regime:
  - low velocities, large diameters
  - $\dot{Q}^* < 10^5$, $Fr_f < 5$, $(L_f / d_F) = O(1)$

- **Momentum**-driven flame regime:
  - high velocities, small diameters
  - $\dot{Q}^* > 10^5$, $Fr_f > 5$, $(L_f / d_F) >> 1$
Main features: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer.
Main features: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Smoke layer composition: hot combustion products mixed with ambient air; depending on fuel type and combustion conditions, may contain significant amounts of soot

- Soot particles
  - Product of incomplete combustion
  - Phase: solid
  - Chemical composition: primarily made of carbon atoms
  - Particle size distribution: from a few nanometers \((10^{-9} \text{ m})\) to several millimeters \((10^{-3} \text{ m})\)
  - Particles geometry: complex shapes (agglomerates of elementary spherical particles)
**Main features:** flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Smoke layer depth: depends on fire size and vent flow rates

Accumulation of smoke near ceiling

Smoke filling and loss of visibility

Fast fire growth and smoke descent to floor
Main features: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Impact of smoke layer: increases (radiation-driven) heat feedback to fuel sources

\[
\begin{align*}
G_{UL} & = \epsilon_{UL} \sigma T_{UL}^4 \\
\epsilon_{UL} & = (1 - \exp(-\kappa_{UL} \times d_{UL})) \\
\kappa_{UL} & = p(x_{H_2O,UL} a_{H_2O}(T) + x_{CO_2,UL} a_{CO_2}(T)) \\
& + C_{soot} f_{v,UL} T_{UL} \\
\end{align*}
\]
Compartment Fires

- **Main features:** flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Impact of smoke layer: increases heat feedback to fuel sources
  - Soot contributes to, and often dominates thermal radiation transport

\[ G_{UL} \approx \sigma T_{soot}^4 \]

- Hot soot: emitter of radiation energy (responsible for yellow glow from flames and thereby responsible for flame luminosity)
- Cold soot: absorber of radiation energy (responsible for flame opacity)
**Compartment Fires**

- **Main features:** flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Impact of smoke layer: increases heat feedback to fuel sources, therefore increases fuel gasification rate and heat release rate
Compartment Fires

- **Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Impact of smoke layer: increases heat feedback to fuel sources, therefore increases fuel gasification rate and heat release rate (fire growth and fire spread)
  - Possible transition to *flashover* (rapid series of ignition events involving all flammable objects/materials present in the fire room)
Compartment Fires

- **Main features:** flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Possible transition to *flashover*: may trigger in turn a transition to *under-ventilated* combustion

*Flames extending out of the compartment of fire origin*
**Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Possible transition to *under-ventilated* combustion
- Flame location: (1) near the fuel source; (2) near the vents
Main features: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Possible transition to under-ventilated combustion
- Classical Burke-Schumann problem (1928): 2 possible regimes

Laminar flame-flow configuration

- Air flows into the compartment
- Fuel is introduced at the base
- Flame forms and rises towards the ceiling
- Walls confine the flame
- Over-ventilated flame with higher heat release rate
- Under-ventilated flame with lower heat release rate

Graph showing flame height (z) as a function of distance (x) for two cases: \( \Phi_a < l \) and \( \Phi_a > l \).
Main features: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer

- Possible transition to *under-ventilated* combustion
- Smoke layer composition: (1) products of complete combustion mixed with air; (2) products of incomplete combustion

(1) Over-ventilated combustion,

(2) Under-ventilated combustion
- **Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Impact of smoke layer: air vitiation as the compartment fire system evolves from well-ventilated to *under-ventilated* combustion
  - Air vitiation reduces the flame intensity and promotes flame extinction
Compartment Fires

- **Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Reduced-scale compartment fire experiments (Utiskul & Quintiere)
    - Vent size: variable width and height
    - Fuel pan: variable diameter

![Diagram of compartment fire setup]

**Inner Size: 40x40x40 cm³**

- Top Vent
- Upper Gas Tube
- Front Wall Thermocouples
- Lower Gas Tube
- Bottom Vent
- Stand to Load Cell with Water Seal
- Heat Flux Gauge
- Adjustable Back Wall
- Heat Flux Gauge
- Center Thermocouple
- Heat Flux Gauge
- Fuel Pan
Compartment Fires

- **Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Reduced-scale compartment fire experiments (Utiskul & Quintiere)
  - Steady under-ventilated fire (flame stabilized at the vents)
**Compartments Fires**

- **Main features**: flow confinement and buoyancy forces lead to the formation of a ceiling-level smoke layer
  - Reduced-scale compartment fire experiments (Utiskul & Quintiere)
  - Unsteady under-ventilated fire leading to complete flame quenching
CFD-Based Compartment Fire Modeling

- **Outline**
  - Overview of Compartment Fire Dynamics
  - **Overview of Fire Modeling**
  - Examples of Compartment Fire Simulations
**Zone modeling**

- A simplified two-layer description of compartment fires
- Main features
  - Computationally cheap (2 control volumes per compartment)
  - System-level view point (unlimited in problem size and scope)
  - Limited domain of application (large use of empirical correlations)

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**Fire Modeling Software**

**Wall Boundaries (ceiling, side walls, floor)**

- Upper layer:
  - Flame zone
  - Fire plume
  - Ceiling smoke layer
- Lower layer:
  - Floor air layer

- *Zone (mass, energy conservation statements)*

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• Zone modeling
  ➢ A simplified two-layer description of compartment fires
  ➢ Developed in the 1980s, acted as a precursor of CFD-based approaches developed in the 1990s
  ➢ Landscape
    • Commercial software: MAGIC (EDF, France)
    • Software with limited distribution: BRI2002 (Building Research Institute, Japan), *etc*
    • Open-source software: CFAST (NIST)
• **CFD modeling**
  - Still a recent (approximately 15 years old) and fast evolving activity
  - Early adoption and now widespread use by different fire safety stakeholders (including researchers, engineers and non-engineers)
  - **Landscape**
    - No commercial software
    - Software with limited distribution: JASMINE (Building Research Establishment, UK), KAMELEON (Norwegian University of Science and Technology/SINTEF, Norway), SMARTFIRE (University of Greenwich, UK), SOFIE (University of Cranfield, UK)
    - Open-source software: FDS (NIST, USA), FireFOAM (FM Global, USA), ISIS (IRSN, France), Code_Saturne (EDF, France)
Fire Modeling Software

- CFD modeling
  - Landscape
    - **RANS models**: JASMINE (Building Research Establishment, UK), KAMELEON (Norwegian University of Science and Technology/SINTEF, Norway), SMARTFIRE (University of Greenwich, UK), SOFIE (University of Cranfield, UK)
    - **LES models**: FDS (NIST, USA), FireFOAM (FM Global, USA), ISIS (IRSN, France), Code_Saturne (EDF, France)
  - **RANS versus LES**
    - RANS limitation: model coefficients are configuration-dependent and require careful calibration work; not well-suited to fire problems that feature a wide variety of configurations
    - LES capability: well-suited to capture the strongly unsteady transient phases observed in fire dynamics as well as the large-scale flow and combustion features that are typical of fire configurations
• **CFD modeling:** fire modeling requires model descriptions of a range of complex multi-physics phenomena
  - Buoyancy-driven turbulent flow
  - Non-premixed combustion
  - Pyrolysis processes
  - Soot formation/oxidation
  - Thermal radiation transport
Fire Modeling (LES)

- **Turbulence modeling**: buoyancy-driven turbulent flow
  - Species mass conservation

\[
\frac{\partial}{\partial t} (\overline{\rho Y_k}) + \frac{\partial}{\partial x_j} (\overline{\rho Y_k u_j}) = - \frac{\partial \lambda_{kj}}{\partial x_j} + \frac{\partial}{\partial x_j} (\rho D_k \frac{\partial Y_k}{\partial x_j}) + \dot{\omega}_k
\]

\[
\lambda_{kj} = \overline{\rho Y_k u_j} - \overline{\rho Y_k u_j}
\]

requires modeling

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**Turbulence modeling:** buoyancy-driven turbulent flow

- Gradient transport model for turbulent fluxes
  \[
  \lambda_{kj} = -\frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_k}{\partial x_j}
  \]
  \(\mu_t\) is a turbulent viscosity
  \(Sc_t\) is a turbulent Schmidt number

- Smagorinsky model: closure expression for the turbulent viscosity
  \[
  \mu_t = \overline{\rho} (C_s \Delta)^2 \sqrt{\frac{1}{2} \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) \left( \frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right)}
  \]
  magnitude of the grid-resolved strain rate tensor

where \(\Delta = (\Delta x_1 \Delta x_2 \Delta x_3)^{1/3}\)
- **Turbulence modeling**: buoyancy-driven turbulent flow
  - Modifications of Smagorinsky model due to buoyancy are usually neglected (grid-resolved buoyancy effects are captured but subgrid-scale effects are not treated)
  - Example of a pool fire configuration

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Fire Modeling (LES)

- **Turbulence modeling**: buoyancy-driven turbulent flow
  - Wall-bounded boundary layer flows feature small-scale physics and represent a special challenge for a CFD treatment
  - Turbulent boundary layer flows feature sharp gradients of flow velocity and temperature at the wall surface
    - These gradients need to be evaluated in order to calculate the wall shear stress and (convective) wall heat flux

\[
\tau_w(x) = \mu \left. \frac{\partial u}{\partial y} \right|_{y=0} ; \quad \dot{q}_{w,c}(x) = -k \left. \frac{\partial T}{\partial y} \right|_{y=0}
\]
**Turbulence modeling:** buoyancy-driven turbulent flow

- Scaling (vertical walls, limit of large Grashof numbers)
  - Viscous sub-layer
    \[ \theta^* = y^* \,, \quad 0 \leq y^* \leq 3 \]
  - Logarithmic layer
    \[ \theta^* = 0.427 \log(y^*) + 1.93 \,, \quad 3 \leq y^* \]
Fire Modeling (LES)

- **Turbulence modeling**: buoyancy-driven turbulent flow
  - Scaling (vertical walls, limit of large Grashof numbers)
      - Wall-resolved treatment (first off-wall fluid node in viscous sub-layer)

\[
\dot{q}''_{w,c} = -k \frac{\partial \tilde{T}}{\partial y}_{w}
\]

Computational grid requirement

\[
0 \leq y_1 \leq 3 \times \frac{(\nu / Pr)^{3/4}}{(\dot{q}''_{w,c} / \rho c_p)^{1/4} (g \beta)^{1/4}}
\]

\[\Delta y_1 \sim 1 \text{ mm}\]
Turbulence modeling: buoyancy-driven turbulent flow

- Scaling (vertical walls, limit of large Grashof numbers)
  M. Hölling & H. Herwig (J. Fluid Mech., 2005)
  - Wall-modeled treatment (first off-wall fluid node in logarithmic layer)

\[
\frac{(h_w - \tilde{h}_1)(\nu / Pr)^{1/4}(g\beta)^{1/4}}{c_p(\dot{q}_{w,c} / \rho c_p)^{3/4}} = 0.427 \log\left(\frac{y_1(\dot{q}_{w,c} / \rho c_p)^{1/4}(g\beta)^{1/4}}{(\nu / Pr)^{3/4}}\right) + 1.93
\]

Mixed thermal boundary condition that relates the wall quantities
\(h_w\) and \(\dot{q}_{w,c}\) to the off-wall enthalpy variable \(\tilde{h}_1\)
**Fire Modeling (LES)**

- **Combustion modeling**: non-premixed turbulent combustion
  - Combustion chemistry: **single-step chemistry model**
    - Fuel composition is often unknown, use a representative surrogate fuel (wood, plastic, foam, fabric, etc)
    - Use a global combustion equation (no detailed chemistry)

\[
C_nH_mO_p + \{n + (m/4) - (p/2) - (v_{CO}/2) - v_{soot}\}O_2 \\
\rightarrow (n - v_{CO} - v_{soot})CO_2 + (m/2)H_2O + v_{CO}CO + v_{soot}C
\]

**Possible extension** to include \( CO \), soot

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**Fire Modeling (LES)**

- **Combustion modeling**: non-premixed turbulent combustion
  - **Infinitely fast chemistry model**: classical mixture fraction-based model
  - Reactive mixture composition

\[
\tilde{Y}_k = \int_0^1 Y_k^{eq}(Z) \tilde{p}(Z) \, dZ
\]

- *state relations* subgridPdf of *Z*
• **Combustion modeling**: non-premixed turbulent combustion
  ➢ Reactive mixture composition: infinitely fast chemistry model
    ➢ Use mixture fraction $Z$ as principal variable and use state relationships to reconstruct the reactive mixture composition once mixture fraction is known

\[
Y_k^{eq}(Z) = 1
\]

![Diagram](image-url)

- $Z_{st} \eta_{CO_2}$
- $Y_{O_2,a}^{eq}$
- $Y_{H_2O}^{eq}$
- $Y_{CO_2}^{eq}$
- $Y_{F}^{eq}$

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• **Combustion modeling:** non-premixed turbulent combustion
  
  ➢ Reactive mixture composition: infinitely fast chemistry model
    
    - Use presumed $\beta$-Pdf (probability density function) model to describe subgrid-scale variations of mixture fraction

\[
\tilde{p}(Z) = \frac{Z^{a-1} (1 - Z)^{b-1}}{\int_0^1 Z^{a-1} (1 - Z)^{b-1} dZ}
\]

where:

\[
a = \tilde{Z} \left( \frac{\tilde{Z} (1 - \tilde{Z})}{(Z_{rms})^2} - 1 \right)
\]

\[
b = (1 - \tilde{Z}) \left( \frac{\tilde{Z} (1 - \tilde{Z})}{(Z_{rms})^2} - 1 \right)
\]

\[
(Z_{rms})^2 = C_{Z_{rms}}^2 \left| \nabla \tilde{Z} \right|^2
\]
• **Combustion modeling:** non-premixed turbulent combustion
  - Reactive mixture composition: infinitely fast chemistry model
    - Solve for spatial/temporal variations of grid-resolved mixture fraction

\[
\frac{\partial}{\partial t} (\rho \bar{Z}) + \frac{\partial}{\partial x_j} (\rho \bar{Z} \bar{u}_j) = \frac{\partial}{\partial x_j} \left( \frac{\mu}{Sc} + \frac{\mu_t}{Sc_i} \frac{\partial \bar{Z}}{\partial x_j} \right)
\]
**Fire Modeling (LES)**

- **Combustion modeling**: non-premixed turbulent combustion
  - **Finite-rate chemistry model**: explicit treatment of mean chemical reaction rates
  - Reactive mixture composition

\[
\hat{Y}_k = \int \int Y^s_{k} (c_1, c_2) \tilde{p}(c_1, c_2) dc_1 dc_2
\]

- State relations
- Subgrid Pdf of Z
Combustion modeling: non-premixed turbulent combustion

- Reactive mixture composition: finite-rate chemistry model
  - Use progress variables $c_1$ and $c_2$ as principal variables and use state relations to reconstruct the mixture composition once $c_1$ and $c_2$ are known
  - Global combustion equation
    \[
    C_nH_mO_p + \left\{ n + \left( \frac{m}{4} - \frac{p}{2} - \frac{v_{CO}}{2} - v_{soot} \right) \right\} O_2 \rightarrow \left( n - v_{CO} - v_{soot} \right) CO_2 + \left( \frac{m}{2} \right) H_2 O + v_{CO} CO + v_{soot} C
    \]
  - Carbon mass decomposition
    \[
    Z = Y_{C_nH_mO_p} + \left( \frac{W_{C_nH_mO_p}}{nW_{CO_2}} \right) Y_{CO_2} + \left( \frac{W_{C_nH_mO_p}}{nW_{CO}} \right) Y_{CO} + \left( \frac{W_{C_nH_mO_p}}{nW_{soot}} \right) Y_{soot}
    \]
    $c_1$ represents fuel mass (THC); $c_2$ represents combined $CO_2$, $CO$ and soot mass
• **Combustion modeling:** non-premixed turbulent combustion
  - Reactive mixture composition: finite-rate chemistry model
    - State relationships give the reactive mixture composition as a function of the principal variables $c_1$ and $c_2$
      \[ Y_{k}^{sr}(c_1, c_2) \]
    - Use presumed Dirac-Pdfs (probability density function) model to describe subgrid-scale variations of $c_1$ and $c_2$
      \[ \tilde{p}(c_1, c_2) \approx \tilde{p}(c_1) \times \tilde{p}(c_2) \approx \delta(c - \tilde{c}_1) \times \delta(c - \tilde{c}_2) \]
Fire Modeling (LES)

- **Combustion modeling:** non-premixed turbulent combustion
  - Reactive mixture composition: finite-rate chemistry model
    - Solve for spatial/temporal variations of grid-resolved reaction progress variables $c_1$ and $c_2$
      
      $$
      \frac{\partial}{\partial t} (\bar{\rho} \bar{c}_1) + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i \bar{c}_1) = \frac{\partial}{\partial x_i} (\bar{\rho} (D + D_t) \frac{\partial \bar{c}_1}{\partial x_i}) - \bar{\omega}_{12}^m
      $$
      
      $$
      \frac{\partial}{\partial t} (\bar{\rho} \bar{c}_2) + \frac{\partial}{\partial x_i} (\bar{\rho} \bar{u}_i \bar{c}_2) = \frac{\partial}{\partial x_i} (\bar{\rho} (D + D_t) \frac{\partial \bar{c}_2}{\partial x_i}) + \bar{\omega}_{12}^m
      $$
      
  - Closure model for the chemical reaction rates: Eddy Dissipation Concept
      
      $$
      \bar{\omega}_{12}^m = \bar{\rho} \times \frac{\min(\bar{Y}_F; \bar{Y}_{O_2} / r_s)}{\tau_t}
      $$

      where $\tau_t = C_t \times (\Delta^2 / \nu_t)$
• **Combustion modeling**: non-premixed turbulent combustion

\[
\dot{q}_{\text{comb}}^m = \bar{\rho} \times \frac{\min(\bar{Y}_F; \bar{Y}_{O_2} / r_s)}{\tau_t} \times \Delta H_{\text{comb}}
\]

where \( \tau_t = C_t \times (\Delta^2 / \nu_t) \)
**Fire Modeling (LES)**

- **Combustion modeling:** non-premixed turbulent combustion
  - Diffusion flame extinction: dominant factor in poorly-ventilated fires
  - Different flame extinction mechanisms
    - Quenching by dilution: flame weakening due to changes in fuel stream or oxidizer stream composition (*e.g.* air vitiation in under-ventilated fires)
    - Thermal quenching: flame weakening due to heat losses (*e.g.* heat losses by convection/conduction, by thermal radiation, by evaporative cooling)
    - Aerodynamic quenching: flame weakening due to flow-induced perturbations (*i.e.* decrease in flame residence time)

---

![Flame](image)

- Fuel side
- Oxidizer side
- \( Y_F < 1 \)
- \( Y_{O_2} < Y_{O_{2,a}} \)
- \( T_{\text{flame}} < T_{\text{ad}}^{\text{flame}} \)
- \( \text{Fuel side} \quad \text{Oxidizer side} \)

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**Combustion modeling**: non-premixed turbulent combustion

- Different flame extinction mechanisms

- Single criterion to predict extinction (laminar flame theory):

  \[
  Da = \frac{\tau_{\text{mixing}}}{\tau_{\text{chemical}}} \leq Da_{\text{critical}}
  \]

  \[
  Da = \frac{\tau_{\text{mixing}}}{\tau_{\text{chemical}}} \sim \frac{1}{\chi_{st}} \exp\left(\frac{T_a}{T_{st}}\right)
  \]

- Two fundamental limits:
  - **Fast mixing limit**: \( Da \) is small because \( \chi_{st} \) is large (e.g., aerodynamic quenching)
  - **Slow mixing limit**: \( Da \) is small because \( T_{st} \) is small (e.g., thermal or dilution quenching)
**Combustion modeling**: non-premixed turbulent combustion

- Flammability map with fuel-air mixing rate and flame temperature as coordinates

\[ T_{st} \]

\[ \delta_c^* \approx 1 \] Extinction limit (AEA theory)

**Engine extinction event**

**Fire extinction event**

**Extinction**
• **Pyrolysis modeling:** description of fuel mass loss rate
  ➢ Different approaches

  ❖ **Empirical:** prescribed fuel mass loss rate (MLR); variable ignition timing

  ❖ **Semi-empirical:** MLR described as perturbation of free-burn values with modifications due to smoke-layer/walls gas-to-solid thermal feedback and air vitiation

  ❖ **Advanced:** MLR predicted from gas-to-solid thermal feedback and finite rate decomposition kinetics
• **Pyrolysis modeling**: description of fuel mass loss rate
  
  - **Finite-rate chemistry model**: explicit treatment of thermal decomposition chemistry
  - Thermal degradation across flammable solid described by a local one-dimensional problem in the direction normal to the exposed solid surface

\[
\rho_s c_s \frac{\partial T_s}{\partial t} = \frac{\partial}{\partial x} \left( k_s \frac{\partial T_s}{\partial x} \right) - \omega_g \frac{\Delta H_{v,g}}{\partial T_s} - m_g c_g \frac{\partial T_s}{\partial x}
\]

- **energy consumed by gasification**
- **convective transport by gas flow**

\[
-k_s \frac{\partial T_s}{\partial x}(0, t) = -\varepsilon G + \varepsilon \sigma (T_s(0, t)^4 - T_\infty^4) + h(T_s(0, t) - T_\infty)
\]

- **heat flux to wall interior (conduction)**
- **radiation**
- **convection**

\( \Delta H_{v,g} \) is the heat required to generate unit mass of volatiles at \( T_s \)

\( G \) is the irradiation from radiant panel, flame, etc
\[ \dot{\omega}_g'' = \rho^0_{vs} x_{vs} A \exp(-E / RT_s) \]

\[ \rho_s = \rho^0_{vs} x_{vs} + \rho^0_c (1 - x_{vs}) \]

\[ \eta_c = \left( \frac{\rho^0_c}{\rho^0_{vs}} \right) \]
**Pyrolysis modeling:** description of fuel mass loss rate

- Finite-rate chemistry model: explicit treatment of thermal decomposition chemistry
- Thermal degradation across flammable solid described by a local one-dimensional problem in the direction normal to the exposed solid surface

\[
\text{virgin solid} \rightarrow \text{volatiles} + \text{char}
\]

\[
\frac{\partial \rho_s}{\partial t} = -\dot{\omega}_g'' \quad \text{mass conservation (solid phase)}
\]

\[
\frac{\partial \rho_g}{\partial t} + \frac{\partial m_g''}{\partial x} = \dot{\omega}_g'' \quad \text{mass conservation (gas phase)}
\]

Fire Modeling (LES)
• **Pyrolysis modeling**: description of fuel mass loss rate
  - Finite-rate chemistry model: explicit treatment of thermal decomposition chemistry
  - Thermal degradation across flammable solid described by a local one-dimensional problem in the direction normal to the exposed solid surface
• Fuel mass loss rate

\[
\dot{\omega}_g(x,t) = \rho_{vs}^0 x_{vs}(x,t) A \exp(-E / RT_s(x,t))
\]

\[
\dot{m}_f(t) = \int_{-\Delta}^{0} \dot{\omega}_g(x,t) dx
\]
• **Pyrolysis modeling**: description of fuel mass loss rate
  - Finite-rate chemistry model: explicit treatment of thermal decomposition chemistry

\[
\begin{align*}
  k^0_{vs} &= k^0_c = 0.126 \text{ W/m} \cdot \text{K} \\
  \rho^0_{vs} &= 663 \text{ kg/m}^3 \\
  \rho^0_c &= 133 \text{ kg/m}^3 \\
  c^0_{vs} &= c^0_c = 2520 \text{ J/kg} \cdot \text{K} \\
  \varepsilon &= 0.9 \\
  A &= 5.250 \times 10^7 \text{ 1/s} \\
  E &= 1.256 \times 10^5 \text{ J/mol} \\
  \Delta H_{v.g} &= 0 \text{ J/kg}
\end{align*}
\]
Pyrolysis modeling: description of fuel mass loss rate

- Finite-rate chemistry model: explicit treatment of thermal decomposition chemistry
- Example: particle board (Novozhilov, Moghtaderi, Fletcher & Kent, Fire Safety J. 27 (1996) 69-84)

\[
k^0_{\text{vs}} = k^0_c = 0.126 \text{ W/m} - \text{K}
\]
\[
\rho^0_{\text{vs}} = 663 \text{ kg/m}^3
\]
\[
\rho^0_c = 133 \text{ kg/m}^3
\]
\[
c^0_{\text{vs}} = c^0_c = 2520 \text{ J/kg} - \text{K}
\]
\[
\varepsilon = 0.9
\]
\[
A = 5.250 \times 10^7 \text{ 1/s}
\]
\[
E = 1.256 \times 10^5 \text{ J/mol}
\]
\[
\Delta H_{v,g} = 0 \text{ J/kg}
\]
Pyrolysis modeling: description of fuel mass loss rate

- Finite-rate chemistry model: explicit treatment of thermal decomposition chemistry
- Unknown parameters: $k_v^0, k_c^0, \rho_v^0, \rho_c^0, c_v^0, c_c^0, \varepsilon_v, \varepsilon_c, A, E, \Delta H_{v,g}$
- Unknown parameters determined by comparison between model predictions and cone calorimeter tests (benchmark quasi-1D tests with controlled irradiation levels and measured fuel mass loss rates) using advanced optimization techniques to minimize the discrepancies
• **Soot modeling**: description of soot emissions
  - Soot emission: leakage of soot particles from the underfire region to the overfire region (across the flame) without oxidation
**Soot modeling**: description of soot emissions

- Smoke point (SP): critical flame length in a laminar jet diffusion flame configuration above which the flame experiences a transition from sooting to smoking conditions.

**Fire Modeling (LES)**

- Sooting flame
- Soot region
- Soot growth
- Soot inception
- Formation of soot precursors
- Soot oxidation
- Soot emission
- Sooting and smoking flame
Fire Modeling (LES)

- **Soot modeling:** description of soot emissions
  - Phenomenological approaches (Moss et al., Lindstedt et al.)
    - Two-variable model; empirical description of fundamental soot formation processes (nucleation, surface growth, coagulation, oxidation)
    - Model parameters are fuel-dependent
    - No PAH chemistry
    - Monodispersed soot particle size distribution

\[
\frac{\partial}{\partial t} \left( \rho Y_{soot} \right) + \frac{\partial}{\partial x_i} \left( \rho u_i Y_{soot} \right) = - \frac{\partial}{\partial x_i} \left( \rho Y_{soot} V_{t,i} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu}{S_c} \frac{\partial Y_{soot}}{\partial x_j} \right) + \dot{\omega}_{s,\text{nucleation}}^m + \dot{\omega}_{s,\text{surface growth}}^m - \dot{\omega}_{s,\text{oxidation}}^m
\]

\[
\frac{\partial}{\partial t} \left( \frac{n_{soot}}{N_A} \right) + \frac{\partial}{\partial x_i} \left( u_i \frac{n_{soot}}{N_A} \right) = - \frac{\partial}{\partial x_i} \left( \frac{n_{soot}}{N_A} V_{t,i} \right) + \frac{\partial}{\partial x_j} \left( \frac{\mu}{\rho S c} \frac{\partial \left( \frac{n_{soot}}{N_A} \right)}{\partial x_j} \right) + \dot{\omega}_{n,\text{nucleation}}^m - \dot{\omega}_{n,\text{coagulation}}^m
\]
**Soot modeling**: description of soot emissions

- Direct numerical simulations (Narayanan, Lecoustre & Trouvé)
  - Flame structure: spatial distribution of soot mass fraction in non-smoking (top) and smoking flames (bottom)
Fire Modeling (LES)

- **Thermal radiation modeling**: description of radiant emissions
  - Thermal radiation transport generally dominates the gas-to-fuel-source thermal feedback; soot particles contribute to and often dominate the fire radiation properties
  - Radiation transport calculated via solving the radiative transfer equation (RTE)
  - Assumptions
    - Non-scattering medium
    - Spectrally-averaged (gray medium) or spectrally-resolved radiation properties
    - Planck mean absorption coefficient function of $CO_2$, $H_2O$ and soot
Thermal radiation modeling: description of radiant emissions

- Radiation transport calculated via solving the RTE
  - Use radiation intensity \([W/m^2]\) as principal variable
    \[I((x,y,z), \mathbf{s})\]
  - Radiative heating/cooling rate \([W/m^3]\)
    \[\dot{q}_{rad}'' = \nabla \cdot \mathbf{q}_R(x, y, z) = \int \nabla I \cdot \mathbf{s} \, d\Omega = \int \frac{dI}{ds} \, d\Omega\]
  - Radiation heat flux vector at surfaces \([W/m^2]\)
    \[\mathbf{q}_R(x, y, z) = \int_{2\pi} I((x, y, z), \mathbf{s}) \mathbf{s} \, d\Omega\]
• **Thermal radiation modeling:** description of radiant emissions
  
  ➢ Radiation transport calculated via solving the RTE
    • Solution method: Discrete Transfer Method (DTM) or Discrete Ordinate Method (DOM)
      
      \[
      \frac{dI}{ds} = \kappa \left( \frac{\sigma T^4}{\pi} \right) - \kappa I
      \]
      
      Emission
      Absorption

  • Mean absorption coefficient [m\(^{-1}\)]
    \[
    \kappa = p(x_{H_2O}a_{H_2O} + x_{CO_2}a_{CO_2}) + \kappa_{soot}
    \]
• **Thermal radiation modeling:** description of radiant emissions
  - Radiation transport calculated via solving the RTE
    - Mean absorption coefficient [m⁻¹]
      \[ \kappa = p(x_{H_2O}a_{H_2O} + x_{CO_2}a_{CO_2}) + \kappa_{soot} \]
    - \( a_{p,i} \) is the Planck mean absorption coefficient for species \( i \) [m⁻¹ atm⁻¹] and is obtained from tabulated data (TNF Workshop web site)
  - \( \kappa_{soot} \) is the soot mean absorption coefficient [m⁻¹]
    \[ \kappa_{soot} = C_{soot} \times f_v T = C_{soot} \times (\rho Y_{soot} / \rho_{soot}) T \]
• **Thermal radiation modeling:** radiation-turbulence interactions (RTI)

  - Radiation transport calculated via solving the RTE

  \[
  \frac{dI}{ds} = \kappa \left( \frac{\sigma T^4}{\pi} \right) - \kappa I
  \]

  \[
  \nabla \cdot \mathbf{q}_R(x, y, z) = \int \nabla I \cdot \mathbf{s} \quad d\Omega = \int \frac{dI}{ds} \quad d\Omega
  \]

  - Mean radiative heating/cooling rate [W/m³]

  \[
  \bar{q}''_{rad} = 4\kappa (\sigma T^4) - \int_{4\pi} \kappa I \quad d\Omega
  \]

  \[
  \text{nonlinear term cannot be approximated by} \quad [4\kappa (\sigma T^4) - \int_{4\pi} \kappa I \quad d\Omega]
  \]
Fire Modeling (LES)

- **Thermal radiation modeling**: description of radiant emissions
  - *Challenges*
    - **Radiation blockage from fuel vapors**: current databases for radiation properties are limited to a small number of chemical species; fuel vapors are often treated as $CH_4$
    - **Turbulence-radiation interactions**: current fire models typically neglect the effects of subgrid-scale fluctuations
  - **Soot modeling**
    - Soot formation/oxidation involve complex processes that are far from being fully understood
    - Fundamental approaches (based on descriptions of soot precursors, soot formation and oxidation mechanisms, soot particle-size distribution) are not ready to provide engineering-level CFD models
    - Need an intermediate semi-empirical approach (*e.g.*, using the smoke point concept)
CFD-Based Compartment Fire Modeling

- Outline
  - Overview of Compartment Fire Dynamics
  - Overview of Fire Modeling
  - Examples of Compartment Fire Simulations
• Fire Dynamics Simulator (FDS)
  - CFD software developed by the Building and Fire Research Laboratory of the National Institute of Standards and Technology (NIST), USA
  - Domain of application: open/enclosure fire simulations (LES formulation; multi-physics: turbulent flow, mixing, combustion, thermal radiation, pyrolysis of liquid/solid fuel, liquid water sprinklers)
    - Limited to low Mach-number flows (no explosion)
    - Low-end engineering projects (ease-of-use, speed)
LES Simulations of Fires

- **Fire Dynamics Simulator (FDS)**
  - Software
    - Public domain ([http://fire.nist.gov/fds](http://fire.nist.gov/fds))
    - Open source (Fortran 90)
    - Large user-group community (Google Code and Google Groups)
    - Parallel (MPI-based)
  - Numerical methods: finite difference scheme (2nd order in space); explicit time integration (2nd order in time); Cartesian grid; multi-block
  - Post-processing capability: Smokeview
LES Simulations of Fires

- **Fire Dynamics Simulator (FDS)**
  - *Example*: simulation of a full-scale test (Dalmarnock fire test, Glasgow, UK, 2006) (Lázaro et al., IAFSS, 2005)
LES Simulations of Fires

- **Fire Dynamics Simulator (FDS)**
  - *Example*: simulation of a full-scale test (Dalmarnock fire test, Glasgow, UK, 2006)

![Heat Release Rate vs time](image)

1. Pre-flashover stage ($t < 300$ s)
2. Flashover ($t = 300$ s)
3. First post-flashover stage ($300 < t < 780$ s) during which the fire size is approximately 3-4 MW
4. First window breakage in the fire room at time $t = 780$ s
5. Second post-flashover stage ($780 < t < 1000$ s) during which the fire size reaches 5-6 MW
6. Second window breakage in the fire room at time $t = 900$ s
7. Decay stage ($t \geq 1000$ s) during which the fire size is observed to decrease
LES Simulations of Fires

- **Fire Dynamics Simulator (FDS)**
  - *Example*: simulation of a full-scale test (Dalmarnock fire test, Glasgow, UK, 2006)

![Global Equivalence Ratio vs time](image)

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(1) Fire becomes under-ventilated (GER ≥ 1) at flashover ($t \approx 300$ s)
(2) Quasi-stoichiometric conditions (GER ≈ 1) during the first post-flashover stage ($300 \leq t \leq 780$ s)
(3) First window breakage at $t = 780$ s results in a slight drop in GER followed by a sharp rise
(4) Fire remains in a transitional regime during the second post-flashover stage ($780 \leq t \leq 1000$ s) and the decay stage ($t \geq 1000$ s).
• Fire Dynamics Simulator (FDS)
  
  Example: simulation of a full-scale test (Dalmarnock fire test, Glasgow, UK, 2006)

\[ t = 236 \text{ s} \]

\[ t = 350 \text{ s} \]

\[ t = 480 \text{ s} \]

\[ t = 810 \text{ s} \]
LES Simulations of Fires

• FireFOAM
  - CFD software developed by FM Global, USA
  - OpenFOAM is a general-purpose advanced CFD solver developed by OpenCFD, UK (http://www.opencfd.co.uk)
    - Library of solvers: LES or RANS approaches for turbulence; low Mach number or compressible flow formulations (fire and explosions)
    - State-of-the-art physical models for LES, turbulent combustion, heat transfer (high-end engineering and research projects)
    - Advanced meshing capabilities: structured or unstructured (polyhedral mesh) computational grid (built-in mesh generation capability)
    - Large user-group community (OpenFOAM)
LES Simulations of Fires

- **FireFOAM**
  - Software
    - Open source (object-oriented C++ environment)
    - Linux OS
    - Massively parallel (MPI-based)
  - Formulation: LES, compressible flow
  - Numerical methods: finite volume scheme (2nd order in space); implicit time integration (2nd order in time); structured or unstructured (polyhedral) grid
  - Post-processing capability: third-party visualization with ParaView (open source)
**LES Simulations of Fires**

- **FireFOAM**
  - Validation test
    - McCaffrey, 1979
    - 30 cm × 30 cm square burner
    - 5 methane flames (scaling)

<table>
<thead>
<tr>
<th>$Q$ [kW]</th>
<th>14</th>
<th>22</th>
<th>23</th>
<th>45</th>
<th>58</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Q^*$</td>
<td>0.19</td>
<td>0.29</td>
<td>0.44</td>
<td>0.60</td>
<td>0.77</td>
</tr>
</tbody>
</table>

$$
\dot{Q}^* = \frac{\dot{Q}}{\rho_\infty c_p T_\infty \sqrt{gDD^2}}
$$

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LES Simulations of Fires

- **FireFOAM**
  - **Mesh**
    - 389k unstructured mesh
    - 24 cells across burner
    - Domain: 3 m × 3 m × 3 m
    - Average time: 13 seconds
LES Simulations of Fires

- FireFOAM
  - Flame height

![Diagram showing flame height vs. HRR with various simulations and equations: $0.2Q^{2/5}$ and $0.08Q^{2/5}$]
LES Simulations of Fires

- **FireFOAM**
  - Time-averaged centerline temperature
LES Simulations of Fires

- **FireFOAM**

  - Time-averaged centerline vertical velocity

![Graph showing V/Q vs. Y/Q^(2/5) for different power inputs](Image)

- 14 kW
- 22 kW
- 33 kW
- 45 kW
- 58 kW
- McCaffrey
• FireFOAM
  ➢ Non-dimensional vertical mass flow rate (air entrainment)
**LES Simulations of Fires**

- **FireFOAM**
  - *Example*: simulation of fire spread in a benchmark parallel panel configuration (Krishnamoorthy *et al.*, *INTERFLAM*, 2010)
  - Validation test
    - Standard intermediate test for materials
    - Heat flux similar to conditions observed in large-scale fires
    - $0.6 \times 0.3 \times 2.4$ m$^3$