Codes à champs pour l'incendie

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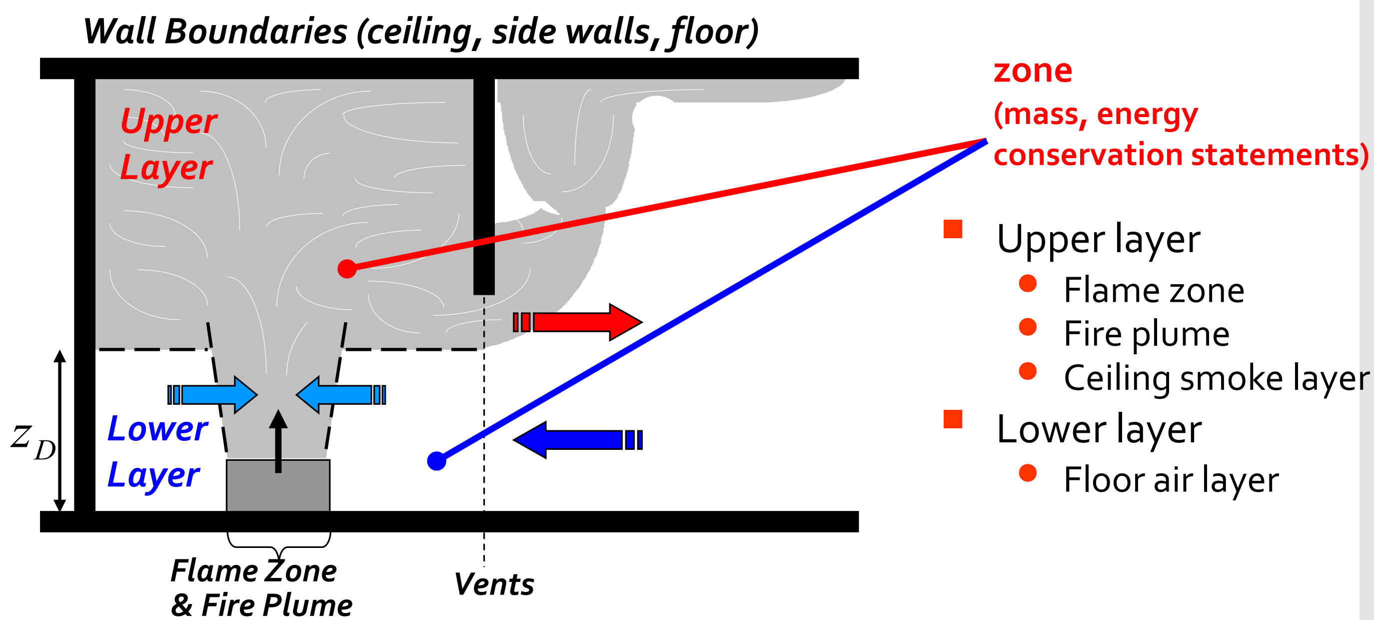
CFD-Based Compartment Fire Modeling

- Outline
  - **Fire modeling approaches**
  - CFD infrastructure
  - Multi-physics modeling

Fire Modeling Approaches

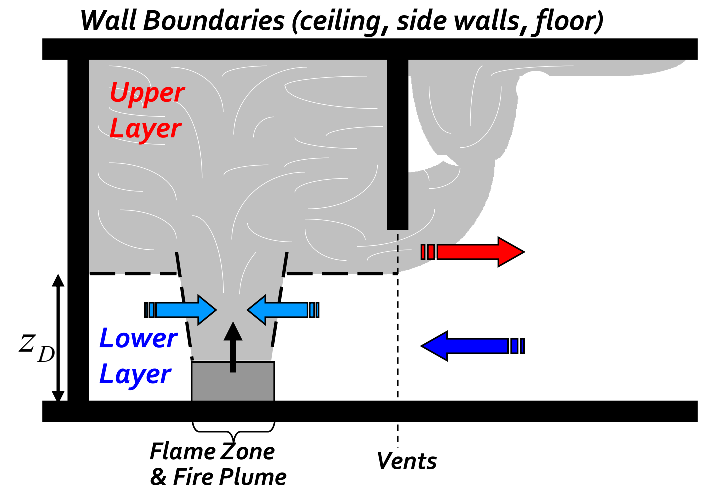
- **Zone modeling**
  - A simplified two-layer description of compartment fires



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

Fire Modeling Approaches

- **Zone modeling**
  - Main features
    - Computationally cheap (two control volumes per compartment)
    - System-level view point (unlimited in problem size and scope)
    - Limited accuracy (use of empirical correlations)

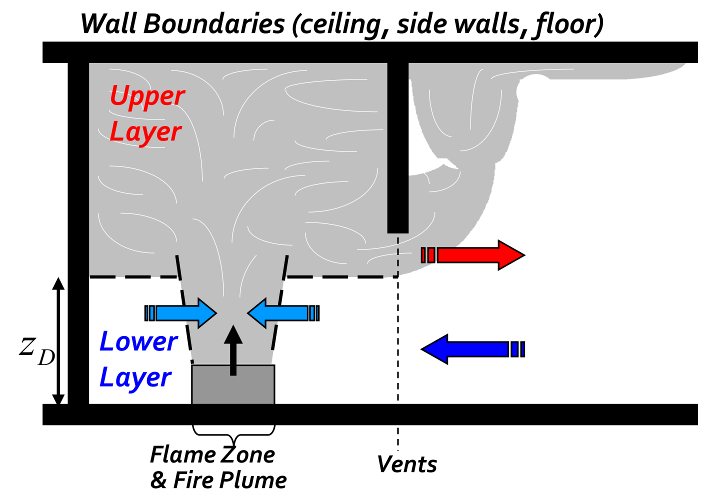


Fire Modeling Approaches

- **Zone modeling**
  - History
    - Developed in the 1980s, acted as a precursor to CFD-based approaches developed in the 1990s
  - Landscape
    - Commercial software: MAGIC (EDF, France)
    - Software with limited distribution: BRI2002 (Building Research Institute, Japan)
    - Open-source software: CFAST (NIST, USA)

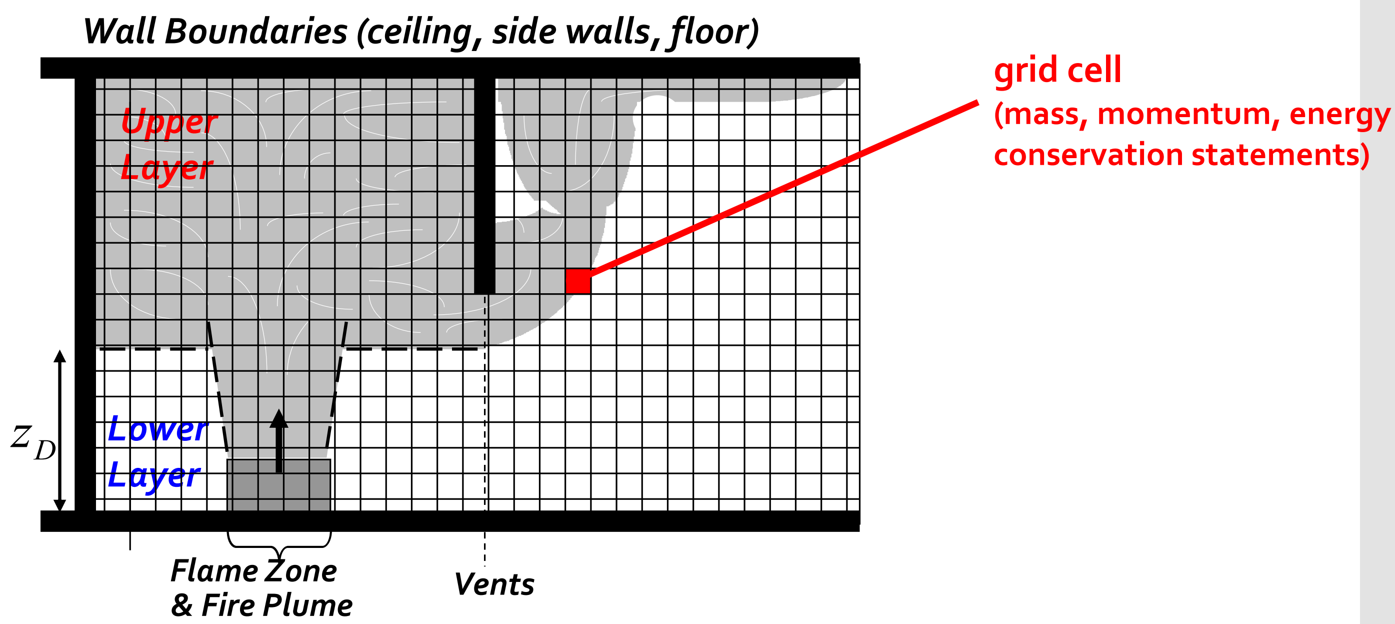
Fire Modeling Approaches

- **Zone modeling**
  - Applications
    - Studies of large/complex building systems (multi-rooms, ventilation system, *etc*)
    - Risk analysis (*e.g.* studies that require 100s/1,000s simulations)



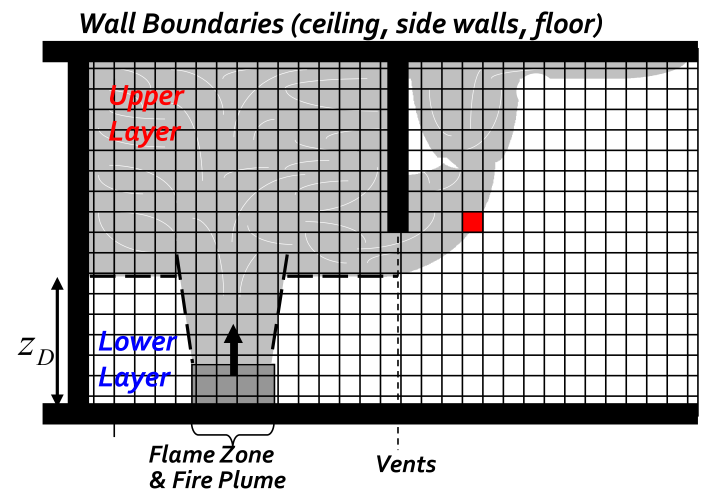
Fire Modeling Approaches

- **CFD modeling**
  - A spatially-resolved description of compartment fires



Fire Modeling Approaches

- **CFD modeling**
  - Main features
    - Computationally expensive (O(10^6) control volumes)
    - Limited view point (in problem size and in scope)
    - Moderate to high/very high accuracy (based on first principles)



Fire Modeling Approaches

- **CFD modeling**
  - History
    - Still a recent (approximately 20-25 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)

Fire Modeling Approaches

- **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), ISIS (IRSN, France)
    - **LES models**: FDS (NIST, USA), FireFOAM (FM Global, USA), ISIS (IRSN, 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

Fire Modeling Approaches

- **CFD modeling**
  - Applications
    - Performance-based design (evacuation performance, smoke management, fire suppression systems, structural resistance, *etc*)
    - Forensic applications
    - Risk analysis
    - Fire-fighter training
    - Sensor-driven real-time emergency management
    - Research (scientific studies of fire dynamics)

CFD-Based Compartment Fire Modeling

- Outline
  - Fire modeling approaches
  - **CFD infrastructure**
  - Multi-physics modeling

CFD Infrastructure

- CFD-based fire modeling (field modeling)
  - A branch in a wider class of simulation tools known as Computational Fluid Dynamics (CFD)
  - CFD infrastructure requires:
    - **Mathematical models** to describe relevant physics
      - ✓ First principles (conservation of mass, momentum, energy)
    - **Numerical algorithms** to solve mathematical models
      - ✓ PDE solvers
      - ✓ Mesh generators
    - **Computer power** to enable numerical algorithms
      - ✓ Massively parallel computers
      - ✓ GPU computers

CFD Infrastructure

- Mathematical modeling (**DNS**)
  - Poinsot & Veynante, "*Theoretical and Numerical Combustion*," 3rd Ed. 2012.

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \frac{\partial}{\partial x_j}(\rho Y_k u_j) = \frac{\partial}{\partial x_j}(\rho D_k \frac{\partial Y_k}{\partial x_j}) + \dot{\omega}_k, \quad 1 \le k \le N_S$$

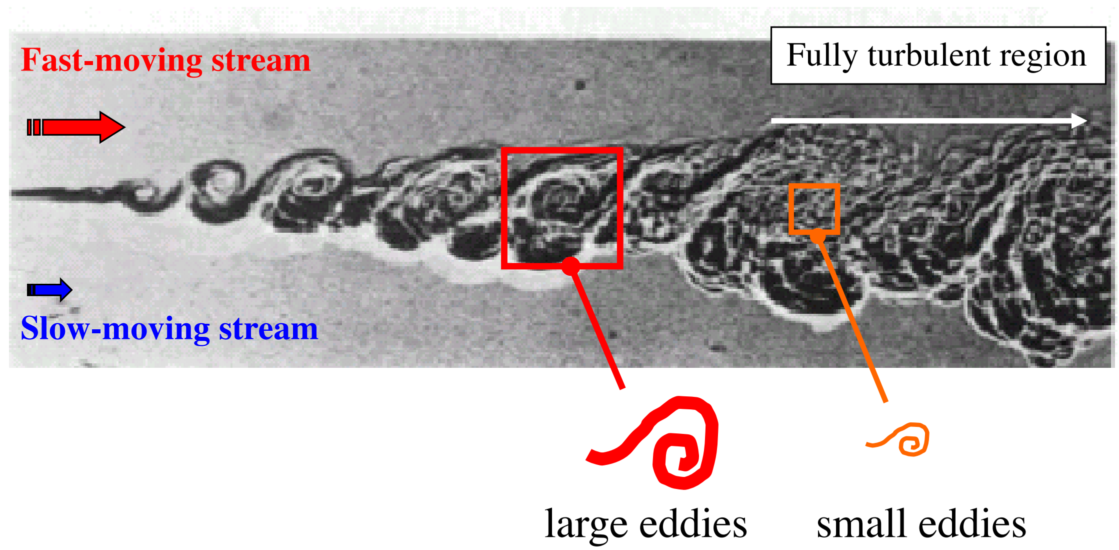
$$\frac{\partial}{\partial t}(\rho u_i) + \frac{\partial}{\partial x_j}(\rho u_i u_j) = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_i, \quad 1 \le i \le 3$$

$$\frac{\partial}{\partial t}(\rho h) + \frac{\partial}{\partial x_j}(\rho h u_j) = \frac{\partial p}{\partial t} + u_j \frac{\partial p}{\partial x_j} + \tau_{ij} \frac{\partial u_i}{\partial x_j} - \frac{\partial q_j}{\partial x_j}$$

$$p = \rho R T (\sum_{k=1}^{N_s} \frac{Y_k}{M_k})$$

CFD Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Turbulence viewed as a multi-scale problem



CFD Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Large eddies (macro-scales)
      - ✓ Turbulent rms velocity (m/s): u'
      - ✓ Integral length scale (m): L_t
      - ✓ Turbulent Reynolds number

$$\mathrm{Re}_t = \frac{\rho u' L_t}{\mu} = \frac{u' L_t}{\nu}$$

    - Small eddies (micro-scales, also called Kolmogorov scales)
      - ✓ Kolmogorov velocity (m/s)

$$v_K = u' \times (\mathrm{Re}_t)^{-1/4}$$

      - ✓ Kolmogorov length scale (m)

$$\eta_K = L_t \times (\mathrm{Re}_t)^{-3/4}$$

CFD Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Example: pool fire, $\dot{Q} = 1 \text{ MW};\ D = 1 \text{ m}$

$$\left.\begin{array}{l} \left.\begin{array}{l} \bar{u}_{CL,\max} \approx 1.9 \times (\dot{Q}/1000)^{1/5} = 7.6 \text{ m/s} \\ u' \approx 0.3 \times \bar{u}_{CL,\max} = 2.3 \text{ m/s} \end{array}\right\} \\ L_t \approx 0.5 \times D = 0.5 \text{ m} \end{array}\right\} \Rightarrow \mathrm{Re}_t = \frac{u' L_t}{\nu} \approx \frac{2.3 \times 0.5}{10^{-4}} \approx 11500$$

$$\Rightarrow \boxed{\eta_K = \frac{L_t}{(\mathrm{Re}_t)^{3/4}} = \frac{0.5}{(11500)^{3/4}} = 0.4 \text{ mm}}$$ (Kolmogorov scaling)

$$\boxed{\Delta x_{DNS} \approx 0.4 \text{ mm}}$$ Grid requirement based on flow

CFD Infrastructure

- Mathematical modeling (DNS)
  - Computational grid requirement
    - Combustion viewed as a numerically stiff problem

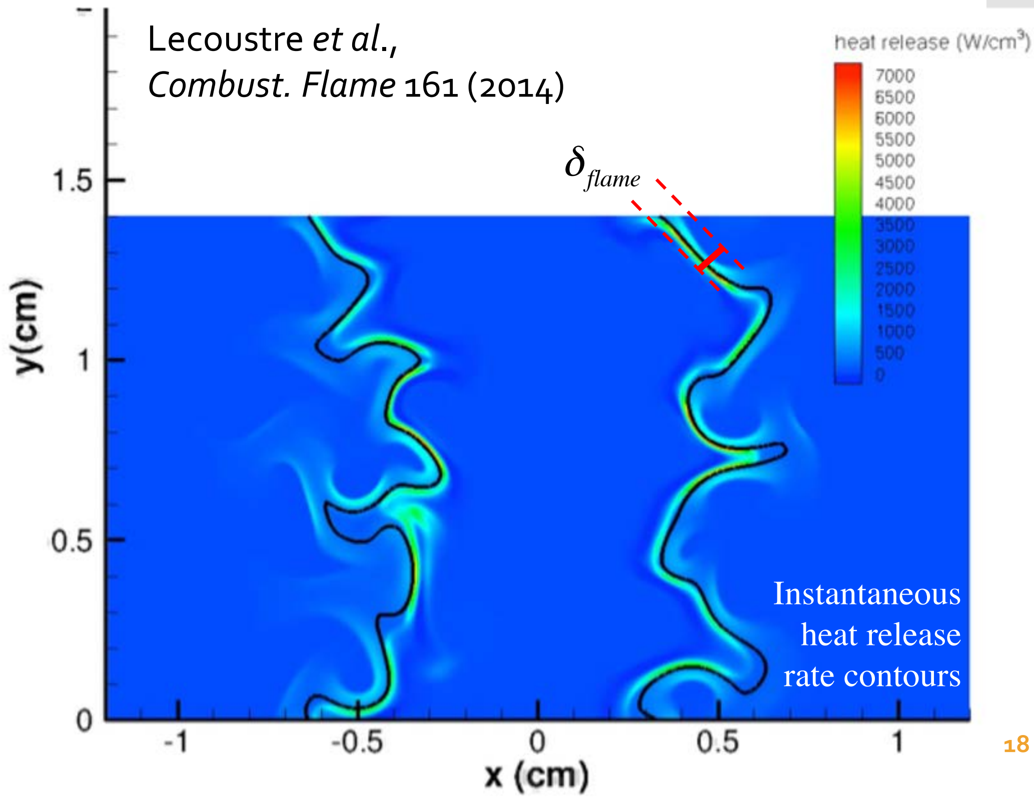
Strained laminar flame theory

$$\delta_{flame} \sim \sqrt{D_{th,st} / \chi_{st}}$$

$$\delta_{flame} \approx 1 \text{ mm}$$

$$\Delta x_{DNS} \approx 0.1 \text{ mm}$$

Grid requirement based on flame



CFD Infrastructure

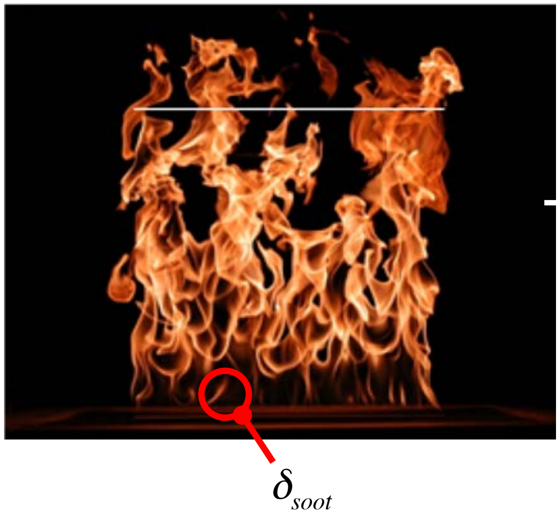
- Mathematical modeling (DNS)
  - Computational grid requirement
    - Thermal radiation viewed as a numerically stiff problem

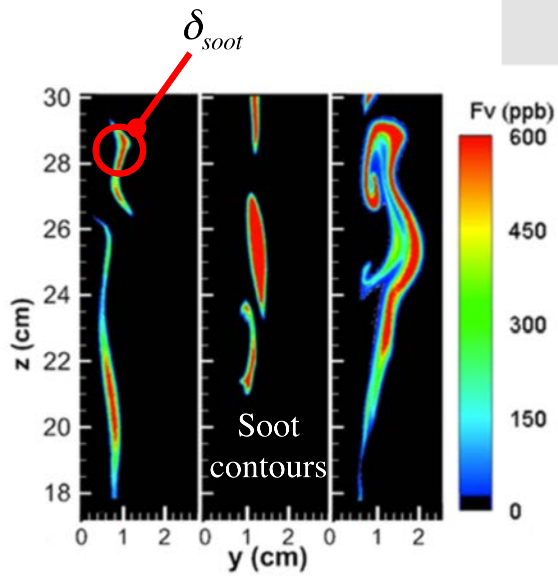
Experimental observations

$\delta_{soot} \sim 1$ mm

$\Delta x_{DNS} \approx 0.1$ mm

Grid requirement based on radiation





Valencia *et al.*
Proc. Combust. Inst. 2016

CFD Infrastructure

- Computational grid requirement
  - Direct Numerical Simulation (DNS)
    - Grid-resolved scales: $L_t, \eta_K, \delta_{flame}, \delta_{soot}$

$$\Delta x_{DNS} \approx \eta_K$$
$$\Delta x_{DNS} \approx (\delta_{flame}/10)$$
$$\Delta x_{DNS} \approx (\delta_{soot}/10)$$

$$\Longrightarrow \boxed{\Delta x_{DNS} = O(0.1\ \mathrm{mm})}$$

CFD Infrastructure

- Mathematical modeling (**LES**)
  - Poinsot & Veynante, "*Theoretical and Numerical Combustion*," 3rd Ed. 2012.

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_j) = 0$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{Y}_k\right) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{Y}_k\tilde{u}_j) = -\frac{\partial \lambda_{kj}}{\partial x_j} + \frac{\partial}{\partial x_j}\overline{(\rho D_k \frac{\partial Y_k}{\partial x_j})} + \overline{\dot{\omega}}_k, \quad 1 \le k \le N_S$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{u}_i\right) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{u}_i\tilde{u}_j) = -\frac{\partial T_{ij}}{\partial x_j} - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\tau}_{ij}}{\partial x_j} + \bar{\rho} g_i, \quad 1 \le i \le 3$$

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{h}) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{h}\tilde{u}_j) = -\frac{\partial Q_j}{\partial x_j} + \frac{\partial \bar{p}}{\partial t} + \overline{u_j \frac{\partial p}{\partial x_j}} + \overline{\tau_{ij}\frac{\partial u_i}{\partial x_j}} - \frac{\partial \bar{q}_j}{\partial x_j}$$

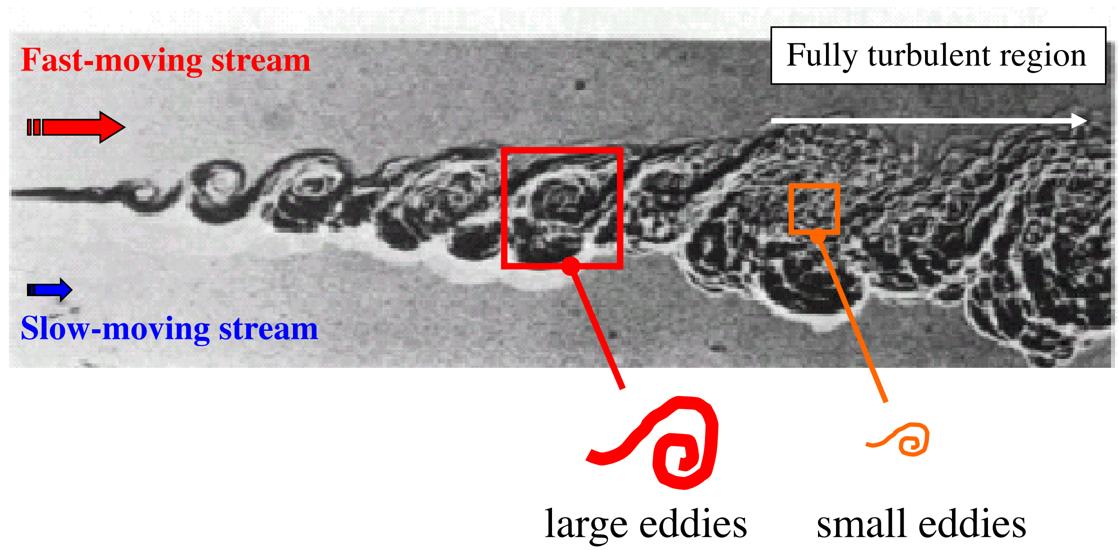
$$\bar{p} = \bar{\rho} R \tilde{T} \sum_{k=1}^{N_s} \frac{\tilde{Y}_k}{M_k} + R \sum_{k=1}^{N_s} \frac{(\overline{\rho T Y_k} - \bar{\rho}\tilde{T}\tilde{Y}_k)}{M_k}$$

CFD Infrastructure

- Mathematical modeling (LES)
  - Mathematical formulation applied to LES-filtered (*i.e.* computational-grid-cell-averaged) quantities; requires models to describe unresolved (subgrid-scale) physics
    - Models to describe turbulent fluxes: $\lambda_{kj}, T_{ij}, Q_j$
    - Models to describe turbulent combustion: $\overline{\dot{\omega}_k}$
    - Models to describe thermal radiation transport: $\overline{q}_j$

CFD Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement
    - Turbulence viewed as a multi-scale problem



CFD Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement (fine-grained LES)
    - Example: pool fire, $\dot{Q} = 1\ \mathrm{MW};\ D = 1\ \mathrm{m}$

$$L_t \approx 0.5 \times D = 0.5\ \mathrm{m}$$

$$\Rightarrow \quad \boxed{\Delta x_{LES} \approx \frac{L_t}{10} = 0.05\ \mathrm{m} \approx 100 \times \Delta x_{DNS}}$$

CFD Infrastructure

- Computational grid requirement
  - Direct Numerical Simulation (DNS)
    - Grid-resolved scales: $L_t, \eta_K, \delta_{flame}, \delta_{soot}$

$$\left.\begin{aligned} \Delta x_{DNS} &\approx \eta_K \\ \Delta x_{DNS} &\approx (\delta_{flame}/10) \\ \Delta x_{DNS} &\approx (\delta_{soot}/10) \end{aligned}\right| \Longrightarrow \boxed{\Delta x_{DNS} = O(0.1\ \mathrm{mm})}$$

  - Large Eddy Simulation (LES)
    - Grid-resolved scales: L_t

$$\boxed{\Delta x_{LES} \approx (L_t/10)}$$

    - Unresolved scales: $\eta_K, \delta_{flame}, \delta_{soot}$

CFD Infrastructure

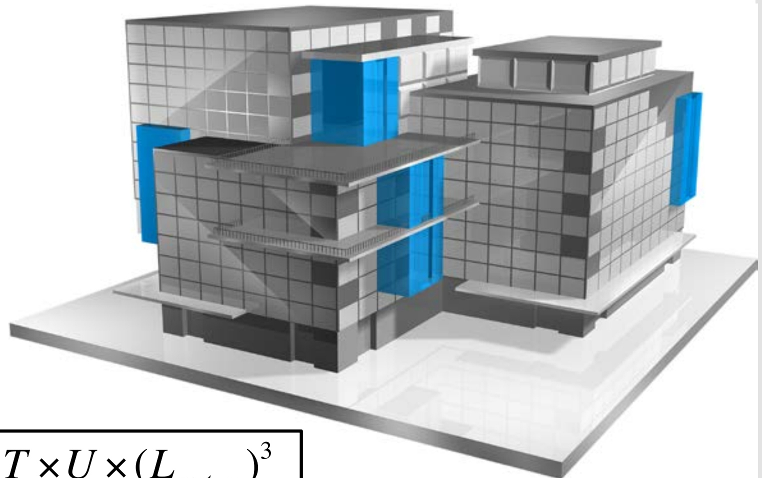
- Mathematical modeling (LES)
  - Computational grid requirement (coarse-grained LES)
    - Example: fire in a large building system

Space: $(L_{system})^3$

$$\frac{\text{CPU cost}}{N_{\Delta t}(N_{\Delta x}N_{\Delta y}N_{\Delta z})} = O(100\mu s)$$

$$N_{\Delta x} \sim N_{\Delta y} \sim N_{\Delta z} = (\frac{L_{system}}{\Delta x})$$

$$N_{\Delta t} = (\frac{T}{\Delta t}) = (\frac{T}{CFL \times (\Delta x / U)})$$



$$\text{CPU cost} \times (\Delta x)^4 = O(100\mu s) \times (\frac{T \times U \times (L_{system})^3}{CFL})$$

CFD Infrastructure

- Mathematical modeling (LES)
  - Computational grid requirement (coarse-grained LES)
    - Example: fire in a large building system

$L_{system} = 50 \text{ m}$

$U = 10 \text{ m/s}$

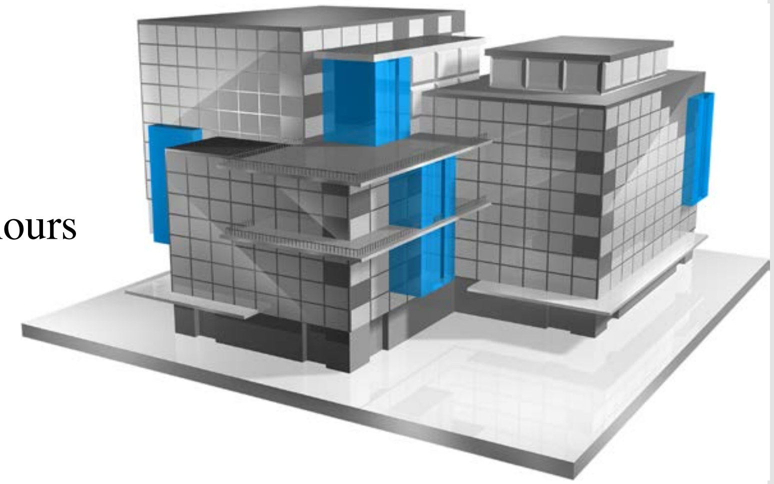
$T = 10 \text{ minutes}$

$\text{CPU cost} = 24 \times 32 \text{ PEs} = 768 \text{ hours}$

$CFL = 0.5$

$\Rightarrow \boxed{\Delta x \sim 0.5 \text{ m}}$

$(N_{\Delta x} N_{\Delta y} N_{\Delta z}) \sim 1 \; Million$



CFD Infrastructure

- Numerical modeling
  - PDE solvers

Model problem

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2}$$

Computational domain

$L_x = 20\,\mathrm{m}$

Initial conditions

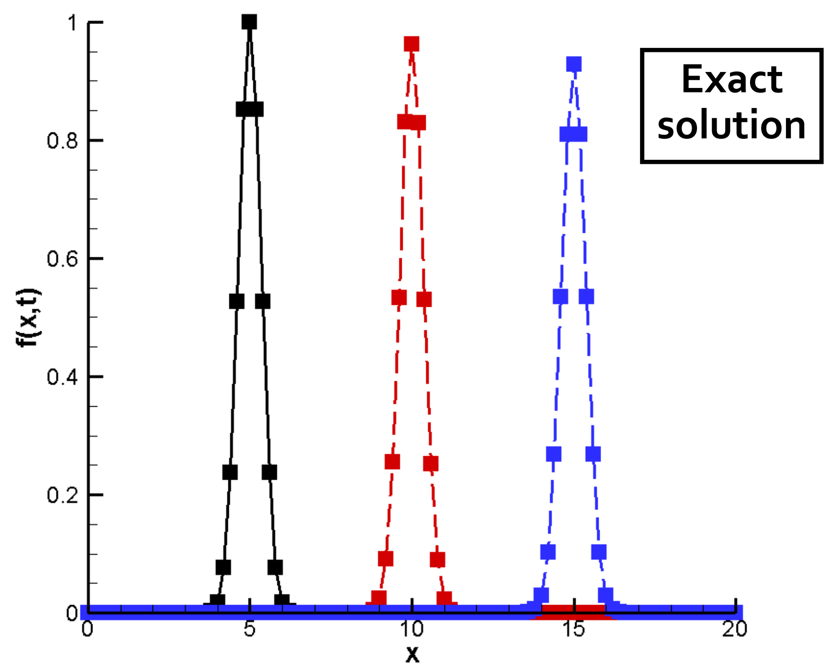
$c(x,t=0) = \exp(-\frac{(x-x_0)^2}{\sigma_0^2})$

$x_0 = 5\,\mathrm{m}\ ;\ \sigma_0 = 0.5\,\mathrm{m}$

Parameters

$u = 1\,\mathrm{m/s}\ ;\ \delta_0 = 2\sigma_0 = 1\,\mathrm{m}$

$\mathrm{Re} = \frac{u \times \delta_0}{D} = 1000\ ;\ D = 10^{-3}\,\mathrm{m^2/s}$



CFD Infrastructure

- Numerical modeling
  - PDE solvers

<u>Model problem</u>

EECD scheme

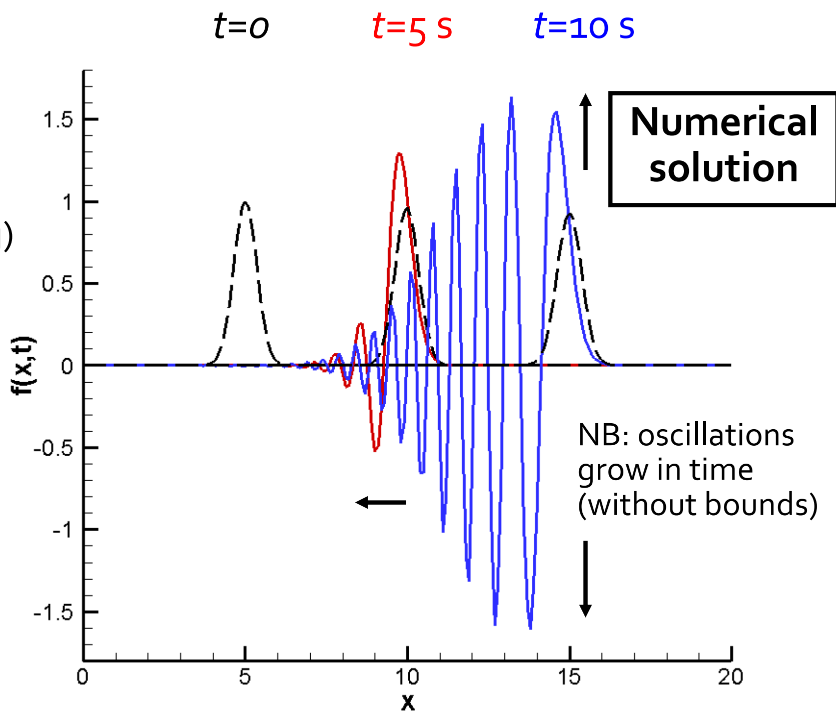
(Euler/explicit, central-differencing)

$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

<u>unstable solution!</u>

(unphysical)



CFD Infrastructure

- Numerical modeling
  - PDE solvers

Model problem

EEUD scheme

(Euler/explicit, upwind-differencing)

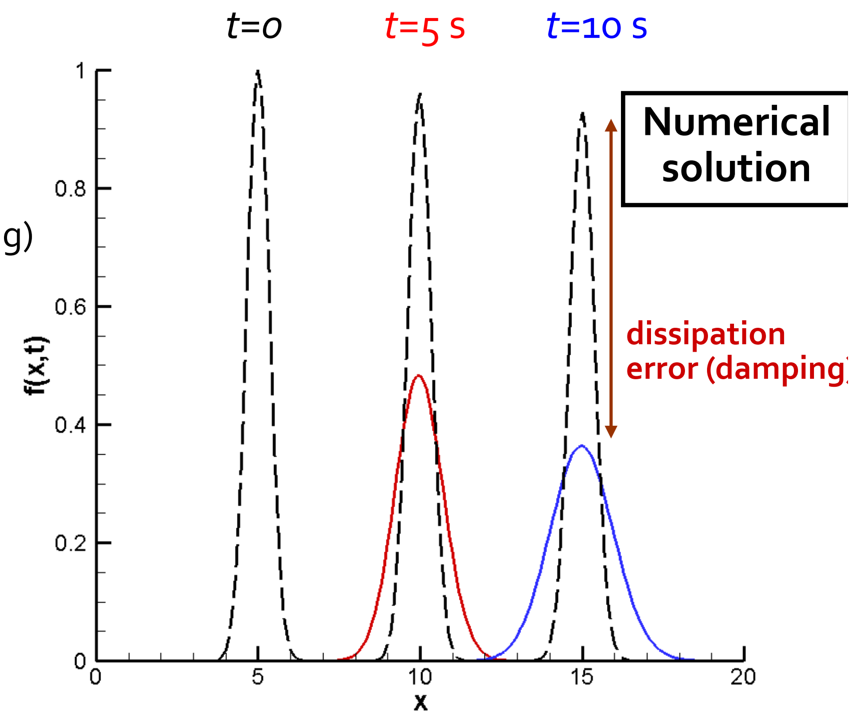
$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

stable solution

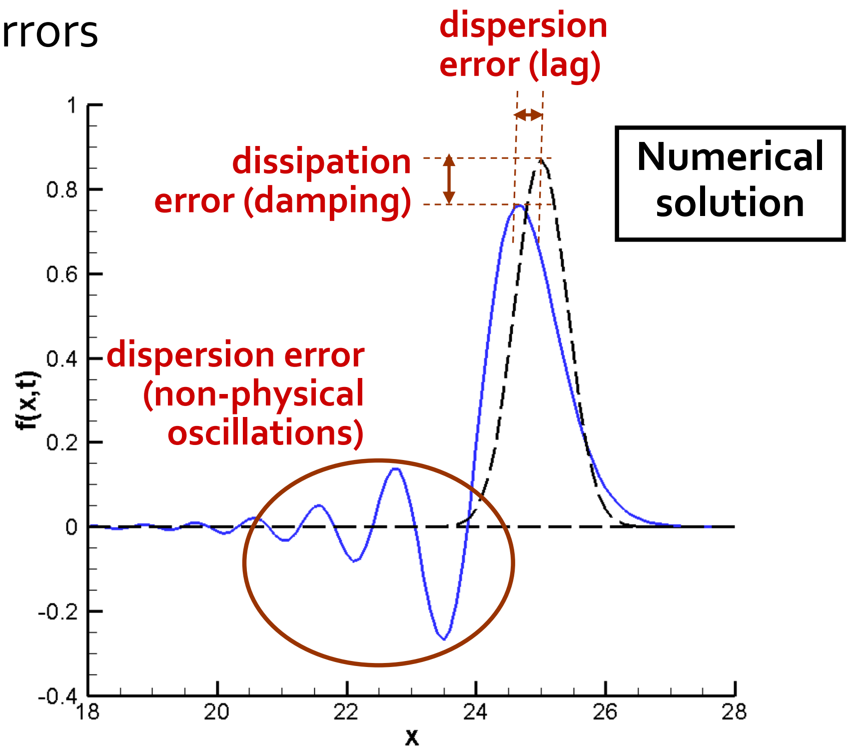
positive solution

(physical but) **inaccurate**



CFD Infrastructure

- Numerical modeling
  - PDE solvers
  - Numerical errors



CFD Infrastructure

- Numerical modeling
  - PDE solvers

<u>Model problem</u>

TVD scheme

(Total Variation Diminishing)

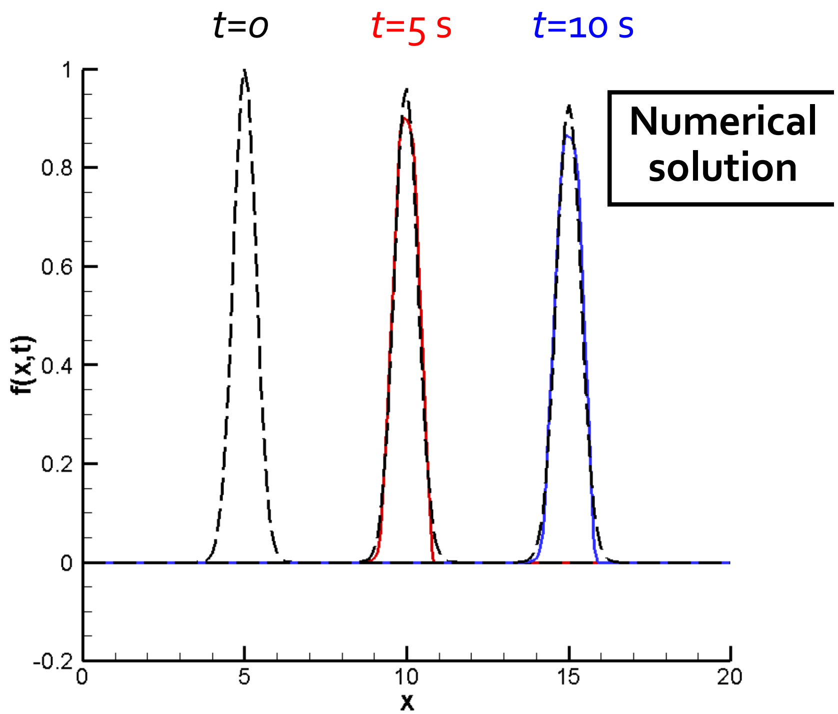
$$\Delta x = (\delta_0 / 10) = 0.1 \text{ m}$$

$$\Delta t = 0.2 \times (\Delta x / u) = 0.02 \text{ s}$$

stable solution

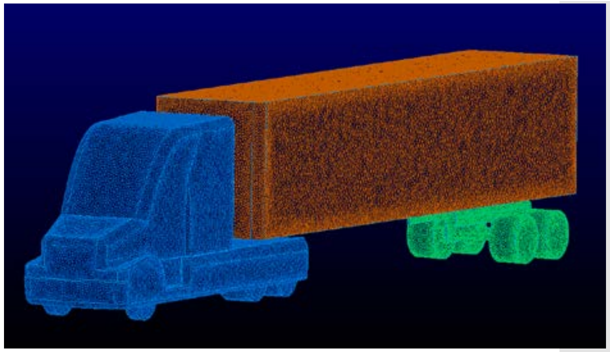
physical and accurate

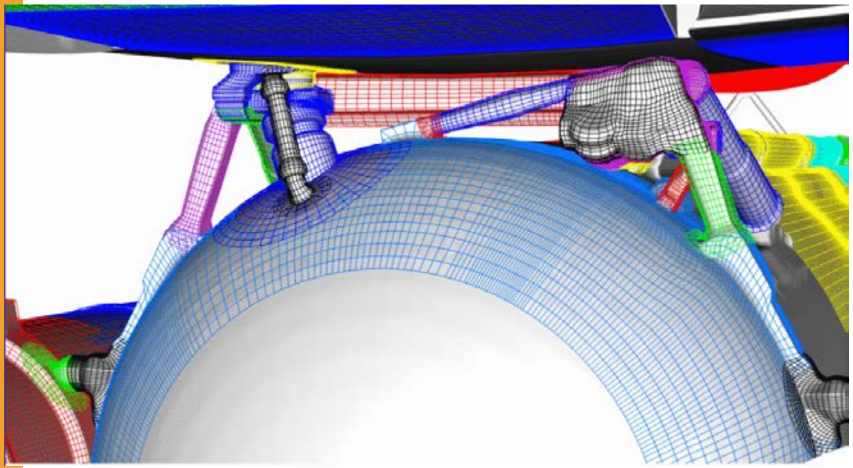
(and positive)



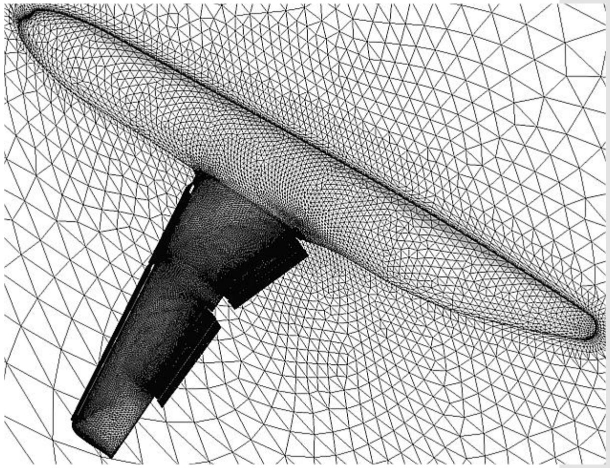
CFD Infrastructure

- Numerical modeling
  - Mesh generators





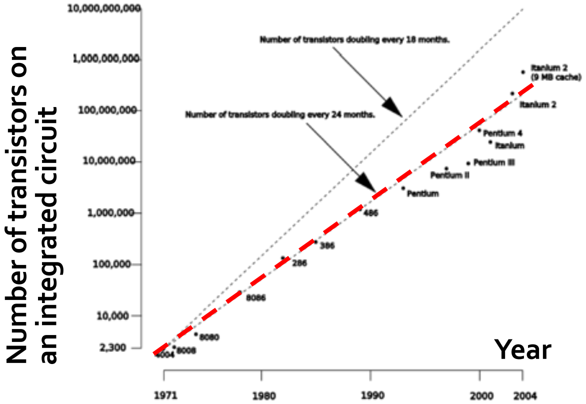
Multiblock-structured grid



Unstructured grid

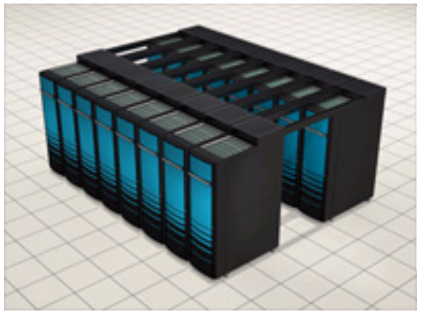
CFD Infrastructure

- Computer power
  - Cyber-infrastructure (CI): Information Technologies for computation, storage, communication, and data processing services, driven by:
    - Fast development of computer and network technologies
    - Dissemination of these technologies on a global scale
    - Rapid decrease in cost (< $1/MFlops)



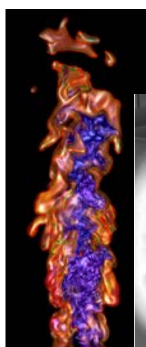
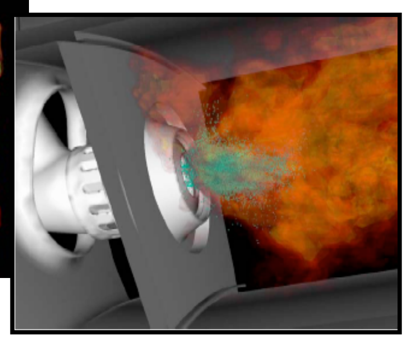
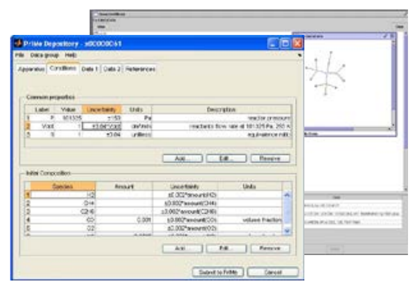
CFD Infrastructure

- Computer power
  - Current status of CI technologies
    - High-performance computing (HPC) facilities (Government Research Laboratories, Universities)
      - ✓ Massively parallel processing systems with computational rates ~ 1 Exa (10^{18}) Flops
    - Small-to-mid-scale computing facilities (Businesses)
      - ✓ Medium-scale parallel computing systems (clusters)
    - Grid infra-structure (coupling of distributed and heterogeneous computational resources and data stores via high-speed networks)
      - ✓ Grid computing



CFD Infrastructure

- Computer power
  - Changes brought by CI technologies
    - Development of *computational research* as a new scientific approach
    - Development of *computational research* as a new engineering approach
    - Development of open-source data and software *digital libraries*
    - Development of distance collaborations and the formation of new *cyber-based communities*


CFD-Based Compartment Fire Modeling

- Outline
  - Fire modeling approaches
  - CFD infrastructure
  - **Multi-physics modeling**

Multi-Physics 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
  - Water spray

Multi-Physics Modeling

- **Turbulence** modeling

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{u}_i\right) + \underbrace{\frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_i\tilde{u}_j\right)}_{\text{grid-resolved convective transport}} = \underbrace{-\frac{\partial T_{ij}}{\partial x_j}}_{\text{subgrid-scale convective transport}} - \frac{\partial \bar{p}}{\partial x_i} + \frac{\partial \overline{\tau_{ij}}}{\partial x_j} + \bar{\rho} g_i$$

$$T_{ij} = \overline{\rho u_i u_j} - \bar{\rho}\tilde{u}_i\tilde{u}_j$$

requires modeling

Multi-Physics Modeling

- **Turbulence** modeling
  - Classical LES treatment: gradient transport model for turbulent fluxes

$$T_{ij} = -\mu_t\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} - \frac{2}{3}\delta_{ij}\frac{\partial \tilde{u}_k}{\partial x_k}\right) + \frac{2}{3}\delta_{ij}\bar{\rho}\tilde{k}_{SGS}$$

μ_t **is a turbulent viscosity**

$$\text{where: } \tilde{k}_{SGS} = \frac{1}{2}\frac{\overline{\rho u_i u_i}}{\bar{\rho}} - \frac{\tilde{u}_i\tilde{u}_i}{2}$$

Multi-Physics Modeling

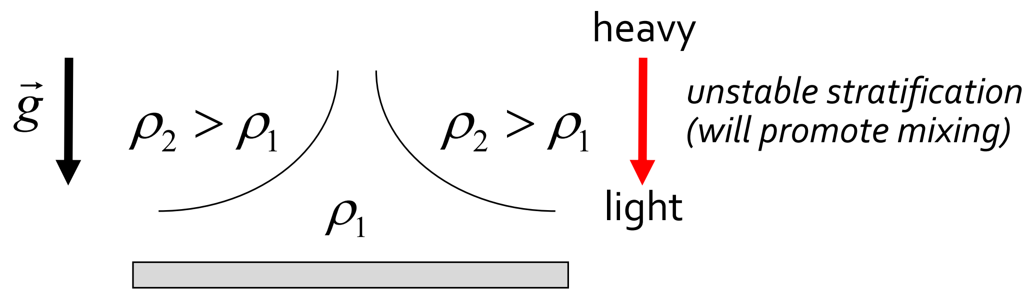
- **Turbulence** modeling
  - Classical LES treatment: closure expression for the turbulent viscosity
    - **Smagorinsky** model

$$\mu_t = \bar{\rho}\left(C_S\Delta\right)^2 \underbrace{\sqrt{\frac{1}{2}\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)\left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i}\right)}}_{\text{magnitude of the grid-resolved strain rate tensor}}$$

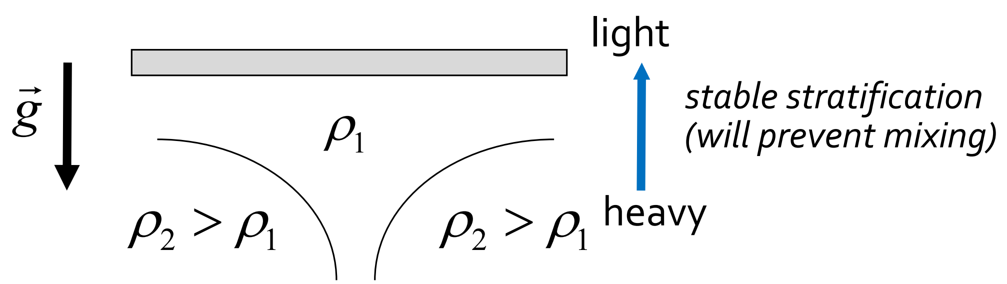
where $\Delta = \left(\Delta x_1 \Delta x_2 \Delta x_3\right)^{1/3}$

Multi-Physics Modeling

- **Turbulence** modeling
  - No treatment of buoyancy effects: Rayleigh-Taylor instabilities; reverse cascade of turbulent kinetic energy
    - Example of a pool fire configuration



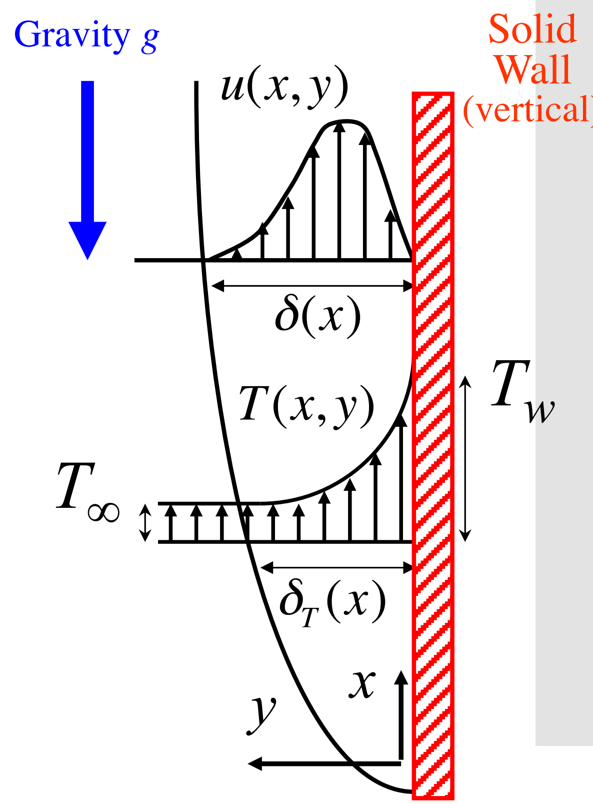
    - Example of a ceiling jet configuration



Multi-Physics Modeling

- **Turbulence** modeling
  - Near-wall treatment
    - 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 wall convective heat flux

$$\tau_w(x) = \mu \left.\frac{\partial u}{\partial y}\right|_{y=0} \ ; \ \dot{q}''_{w,c}(x) = -k \left.\frac{\partial T}{\partial y}\right|_{y=0}$$

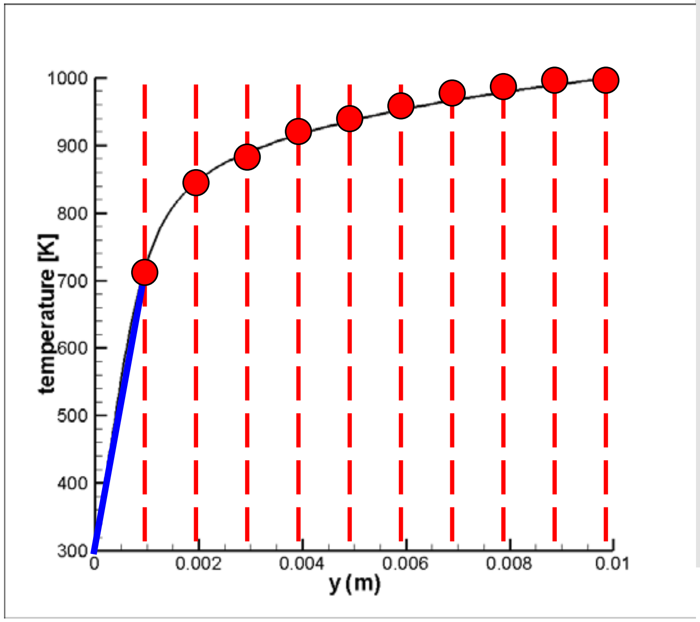


Multi-Physics Modeling

- **Turbulence** modeling
  - Near-wall treatment
    - **Wall-resolved LES**: fine-grained simulations in which the wall gradients are captured by the computational grid

$$\Delta y = O(1\ \mathrm{mm})$$

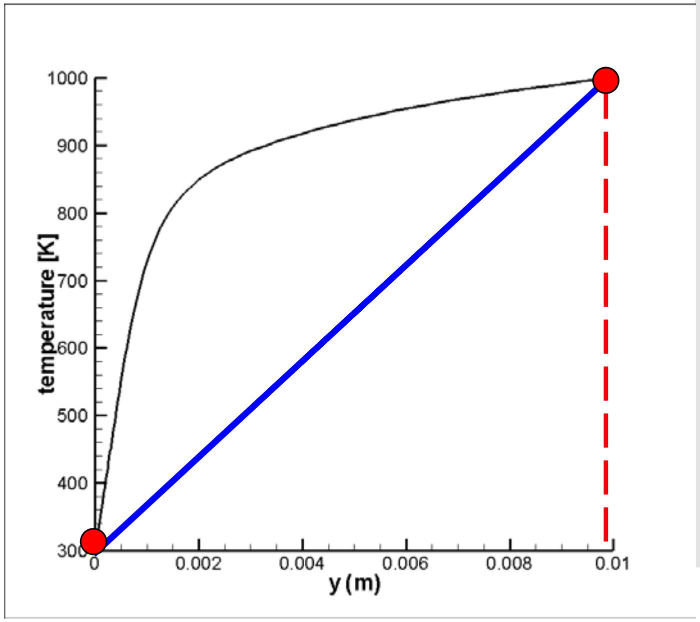
$$\dot{q}''_{w,c} = -k \left.\frac{\partial T}{\partial y}\right|_{y=0}$$



Multi-Physics Modeling

- **Turbulence** modeling
  - Near-wall treatment
    - **Wall-modeled LES**: coarse-grained simulations in which the wall gradients are not captured by the computational grid (*i.e*. are unresolved) and are reconstructed through a wall model

$\dot{q}''_{w,c}$?



Multi-Physics Modeling

- **Combustion** modeling

$$\frac{\partial}{\partial t}(\bar{\rho}\tilde{Y}_k) + \frac{\partial}{\partial x_j}(\bar{\rho}\tilde{Y}_k\tilde{u}_j) = -\frac{\partial \lambda_{kj}}{\partial x_j} + \frac{\partial}{\partial x_j}\overline{(\rho D_k \frac{\partial Y_k}{\partial x_j})} + \underbrace{\overline{\dot{\omega}'''_k}}_{\substack{\text{mass reaction rate} \\ \text{(grid-scale} \\ \text{and subgrid-scale)}}}$$

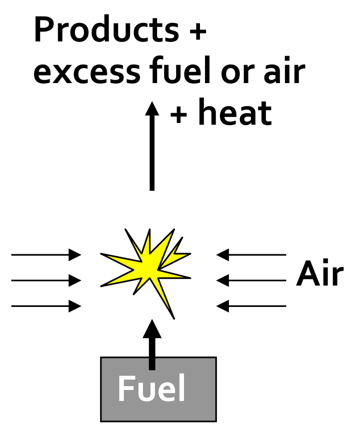
requires modeling

Multi-Physics Modeling

- **Combustion** modeling
  - Non-premixed turbulent combustion
    - Fuel composition is often unknown in fire problems, use a representative surrogate fuel (wood, plastic, foam, fabric, *etc*)
    - Global combustion equation (no chemistry)

$$C_nH_mO_p + \{n + (m/4) - (p/2) - (\nu_{CO}/2) - \nu_{soot}\}O_2$$
$$\rightarrow (n - \nu_{CO} - \nu_{soot})CO_2 + (m/2)H_2O + \underbrace{\nu_{CO}CO}_{\text{carbon monoxide}} + \underbrace{\nu_{soot}C}_{\text{soot}}$$

possible extension to include *CO*, soot



Multi-Physics Modeling

- **Combustion** modeling
  - Non-premixed turbulent combustion
    - **Eddy Dissipation Concept** model: rate of combustion is limited by fuel-air mixing; explicit treatment of the chemical reaction rates

$$\overline{\dot{\omega}_F'''} = \overline{\rho} \times \frac{\min(\tilde{Y}_F ; \tilde{Y}_{O_2} / r_s)}{\tau_t} \quad \text{where} \quad \tau_t = C_{\tau_t} \times (\frac{\overline{\rho}\Delta^2}{\mu_t})$$

$$\overline{\dot{q}_{comb}'''} = \overline{\rho} \times \frac{\min(\widetilde{Y}_F ; \widetilde{Y}_{O_2} / r_s)}{\tau_t} \times \Delta H_{comb}$$

Multi-Physics Modeling

- **Combustion** modeling
  - Diffusion flame extinction
    - Different mechanisms
      - ✓ *Quenching by dilution*: flame weakening du to changes in fuel stream or oxidizer stream composition (*e.g.* air vitiation in under-ventilated fires)

Flame

Fuel side | Oxidizer side

$Y_F < 1$ | $Y_{O_2} < Y_{O_{2,a}}$

      - ✓ *Thermal quenching*: flame weakening due to heat losses (*e.g.* heat losses by thermal radiation or by evaporative cooling)

Flame

Fuel side | Oxidizer side

$T_{flame} < T_{flame}^{ad}$

      - ✓ *Aerodynamic quenching*: flame weakening due to flow-induced perturbations (*i.e.* decrease in flame residence time)

Flame

Fuel side | Oxidizer side

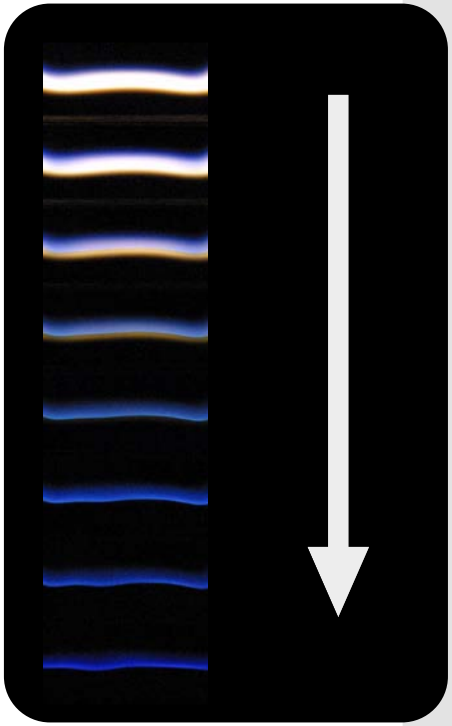
Multi-Physics Modeling

- **Combustion** modeling
  - Diffusion flame extinction
    - Single criterion to predict extinction (laminar flame theory)

$$Da = \frac{\tau_{mixing}}{\tau_{chemical}} \leq Da_{critical}$$

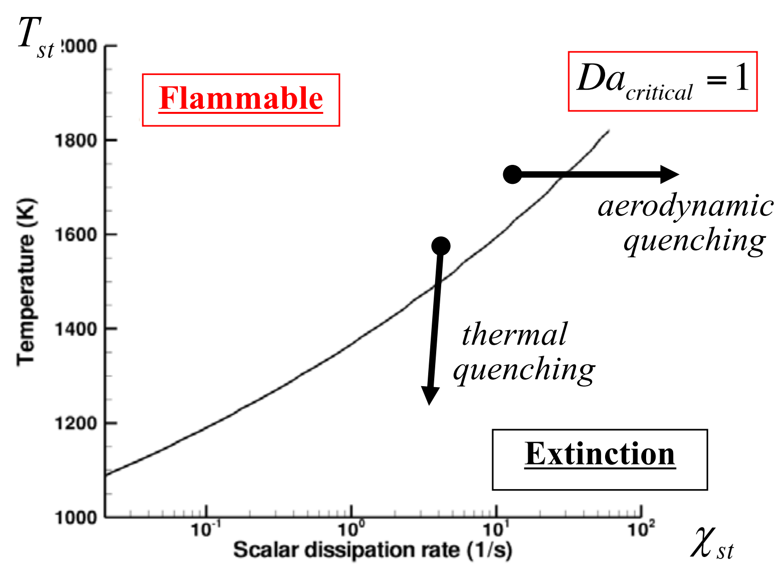
$$Da = \frac{\tau_{mixing}}{\tau_{chemical}} \sim \frac{(1/\chi_{st})}{\exp(T_a/T_{st})}$$

    - Two fundamental limits:
      - ✓ *Fast mixing limit*: *Da* is small because χ_{st} is large (*e.g.* aerodynamic quenching)
      - ✓ *Slow mixing limit*: *Da* is small because T_{st} is small (*e.g.* thermal/dilution quenching)



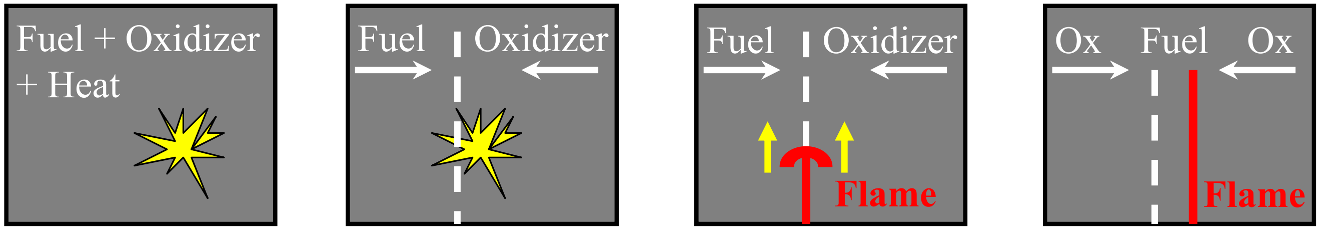
Multi-Physics Modeling

- **Combustion** modeling
  - Diffusion flame extinction
    - Flammability map with fuel-air mixing rate and flame temperature as coordinates



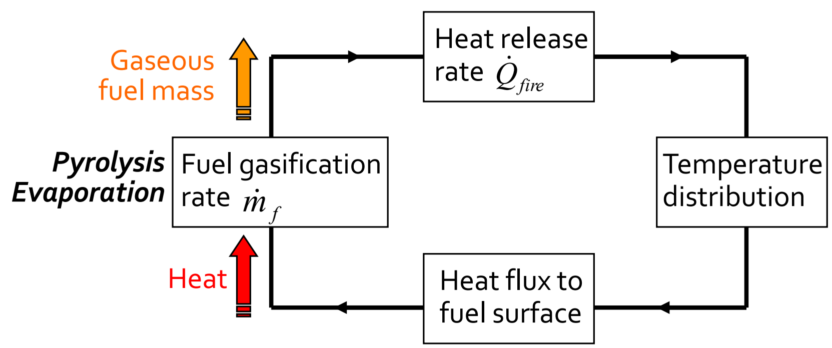
Multi-Physics Modeling

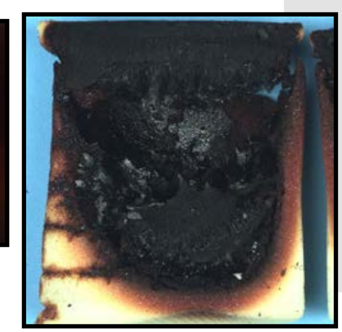
- **Combustion** modeling
  - Diffusion flame extinction
    - Flame extinction may lead to full extinction or to flame *re-ignition*
    - Different mechanisms for flame re-ignition
      - ✓premixed auto-ignition
      - ✓non-premixed auto-ignition
      - ✓edge flame propagation
      - ✓flame-flame interaction



Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Different approaches
      - ✓ ***Empirical***: prescribed MLR; variable ignition timing
      - ✓ *Semi-empirical*: MLR described as perturbation of free-burn values with modifications due to smoke/walls thermal feedback and air vitiation
      - ✓ ***Advanced***: MLR predicted from gas-to-solid thermal feedback and finite rate decomposition kinetics



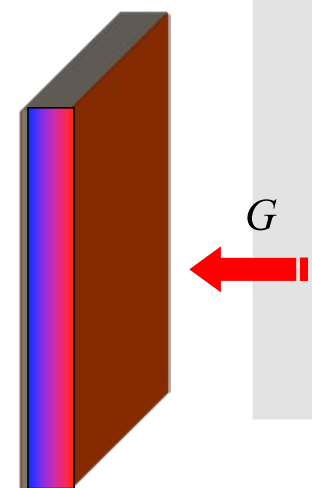


Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Thermal degradation across flammable solid described by a local 1D problem in the direction normal to the exposed solid surface

$$\underbrace{-k_s \frac{\partial T_s}{\partial x}(0,t)}_{\substack{\text{heat flux to solid interior} \\ \text{(conduction)}}} = \underbrace{-\varepsilon G + \varepsilon \sigma (T_s(0,t)^4 - T_\infty^4)}_{\text{radiation}} + \underbrace{h(T_s(0,t) - T_\infty)}_{\text{convection}}$$

thermal feedback
(challenge: need to be evaluated accurately)



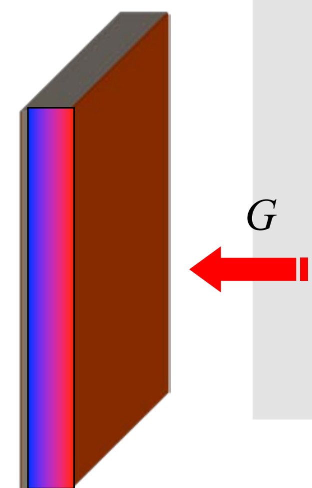
Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Single-step chemistry (and porosity << 1)

$$\underbrace{\text{virgin solid}}_{1\text{ kg}} \rightarrow \underbrace{\text{volatiles}}_{\eta_g = 1-\eta_c} + \underbrace{\text{char}}_{\eta_c}$$

$$\dot{\omega}_g''' = (1-\eta_c)(\rho_s Y_{vs}) A \exp(-E/RT_s)$$

$$\rho_s \equiv \frac{m_s}{V_s + V_g} \qquad Y_{vs} \equiv \frac{m_{vs}}{m_s}$$



Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Governing equations (**without volume change**)

$$\frac{\partial \rho_s}{\partial t} = -\dot{\omega}_g'''$$

mass conservation (solid phase)

$$\frac{\partial \rho_g}{\partial t} + \frac{\partial \dot{m}_g''}{\partial x} = \dot{\omega}_g'''$$

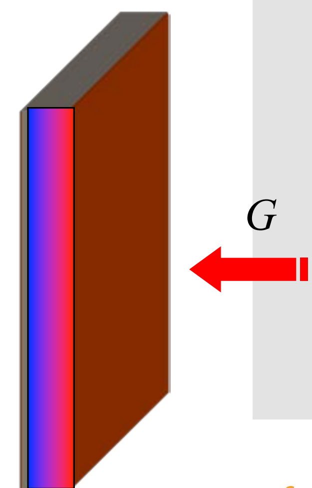
mass conservation (gas phase)

$$\frac{\partial}{\partial t}(\rho_s h_s) = \frac{\partial}{\partial x}\left(k_s \frac{\partial T_s}{\partial x}\right) - \dot{\omega}_g''' \Delta H_v$$

energy conservation (solid phase)

$$h_s = \int_{T_0}^{T_s} c_s(T)\, dT$$

ΔH_v is the heat required to generate unit mass of volatiles at T_s

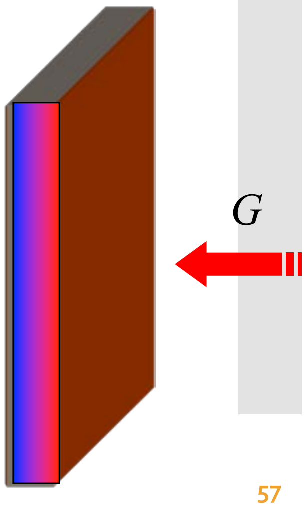


Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Governing equations (**with volume change**)

(Lautenberger & Fernandez-Pello, *Proc. 10th Intl. Symp. Fire Safety Science*, IAFSS, 2011; see also http://code.google.com/p/gpyro/)

$$\begin{cases} \frac{\partial}{\partial t}(\rho_s \Delta x) = -\dot{\omega}_g''' \Delta x \\ \frac{\partial}{\partial t}(\rho_s h_s \Delta x) = \frac{\partial}{\partial x}(k_s \frac{\partial T_s}{\partial x}) \Delta x - \dot{\omega}_g''' \Delta H_v \Delta x \\ \rho_c^0 \frac{\partial}{\partial t}(\Delta x) = \frac{\eta_c - (\rho_c^0 / \rho_{vs}^0)}{1 - \eta_c} \dot{\omega}_g''' \Delta x \end{cases}$$



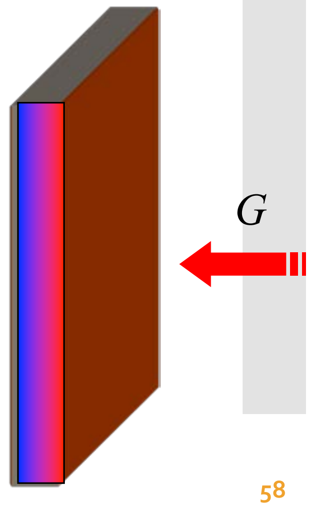
Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Fuel mass loss rate

$$\underbrace{\text{virgin solid}}_{1\text{ kg}} \rightarrow \underbrace{\text{volatiles}}_{\eta_g = 1-\eta_c} + \underbrace{\text{char}}_{\eta_c}$$

$$\dot{\omega}_g''' = (1-\eta_c)(\rho_s Y_{vs}) A \exp(-E/RT_s)$$

$$\boxed{\dot{m}_f''(t) = \int_{-\Delta(t)}^{0} \dot{\omega}_g'''(x,t)\, dx}$$



Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Example: PVC (Ghorbani & Trouvé, model from Stoliarov)

Virgin Material Properties		
ρ	1729.7	kg/m³
c	1111.3	J/kg-K
k	0.17	W/m-K
ε	0.9	

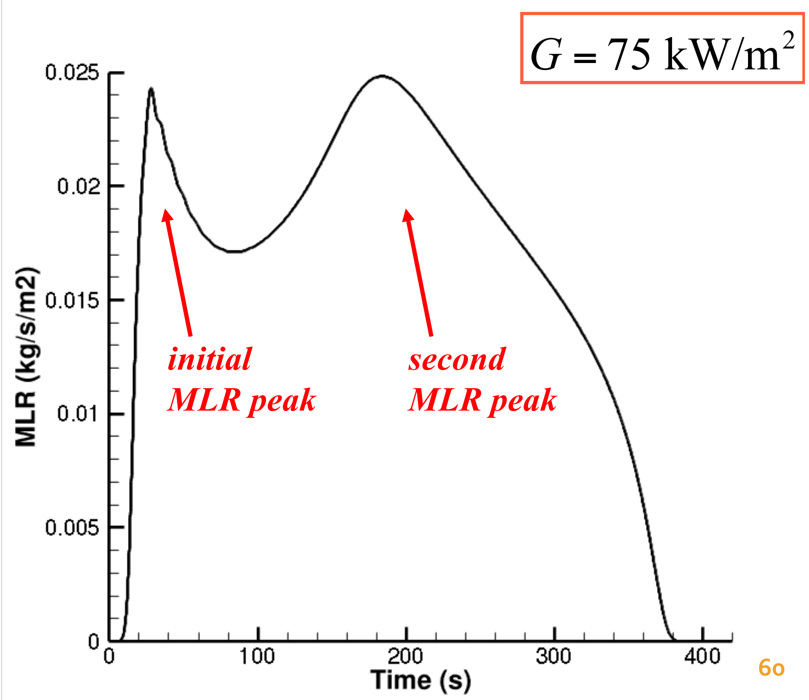
Char Material Properties		
ρ	397.8	kg/m³
c	3894.3	J/kg-K
k	0.10	W/m-K
ε	0.9	
η_C	0.23	

Reaction Parameters		
ΔH_v	3.79E+05	J/kg
A	2.98E+13	1/s
E	1.93E+5	J/mol

Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Example: PVC (Ghorbani & Trouvé, model from Stoliarov)

$$\Delta(t=0) = 0.5 \text{ cm}$$
$$h(x=0) = 10 \text{ W/m}^2\text{/K}$$
$$T_g(x=0) = 293 \text{ K}$$
$$x = \Delta\text{: adiabatic surface}$$
$$\Delta x(t=0) = 100\ \mu\text{m}$$
$$\Delta t = 0.1\ s$$
$$\chi = 1$$



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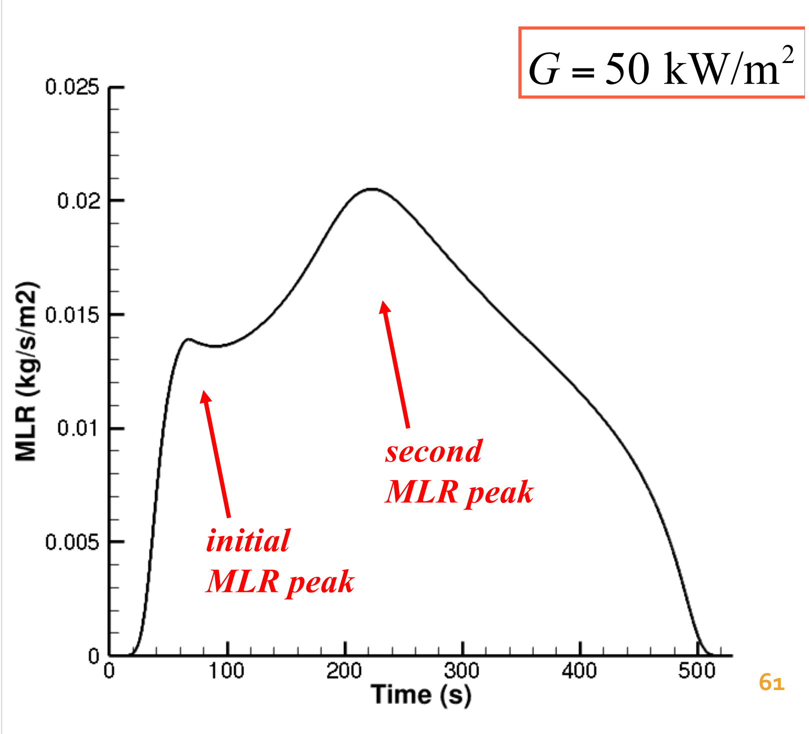

Multi-Physics Modeling

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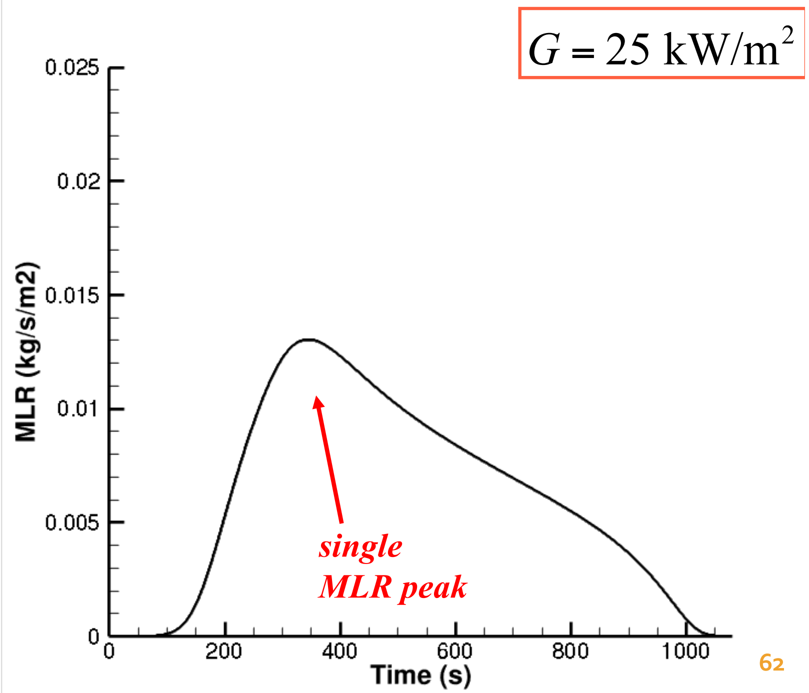
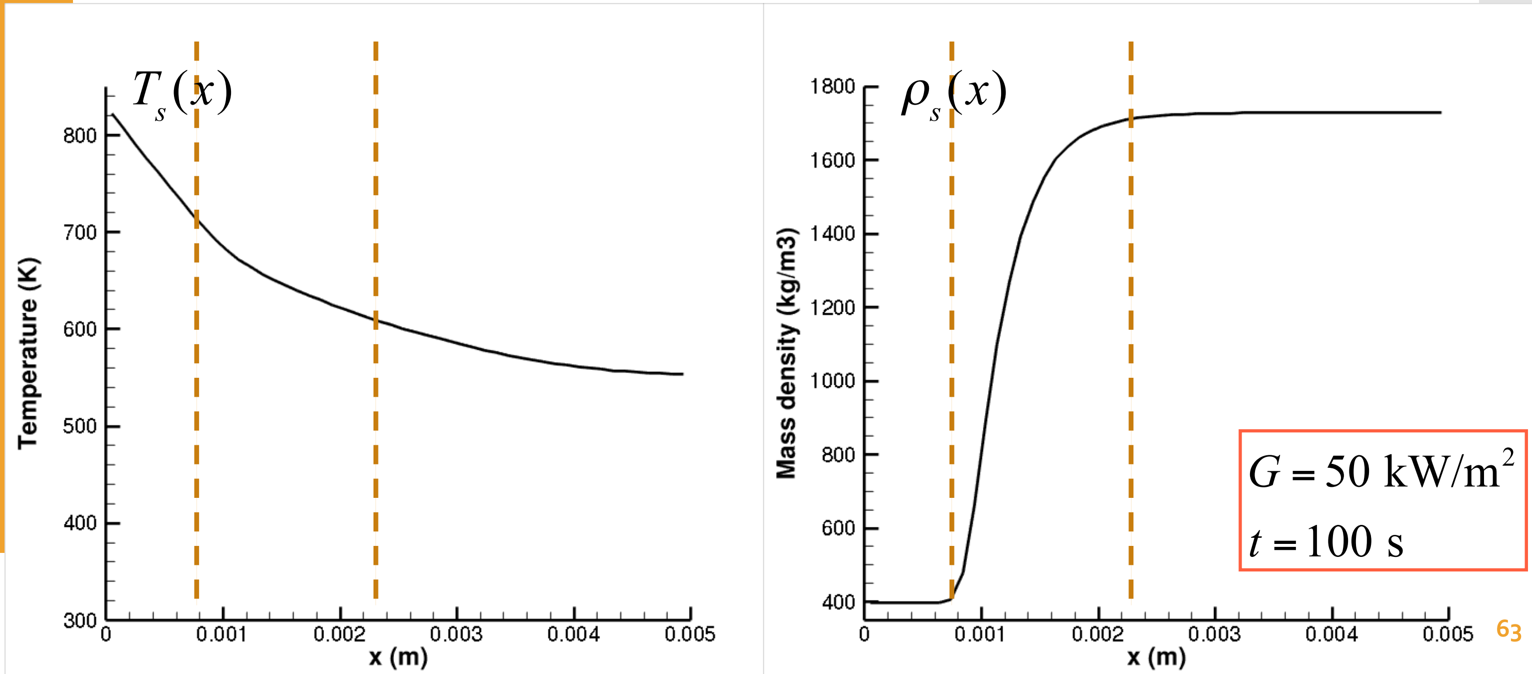


Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Example: PVC (Ghorbani & Trouvé, model from Stoliarov)

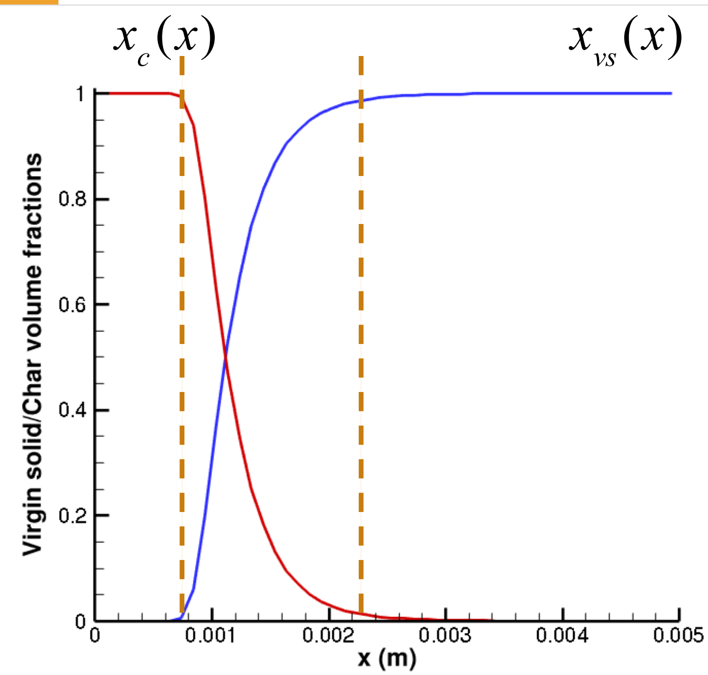
Instantaneous spatial variations inside PVC sample

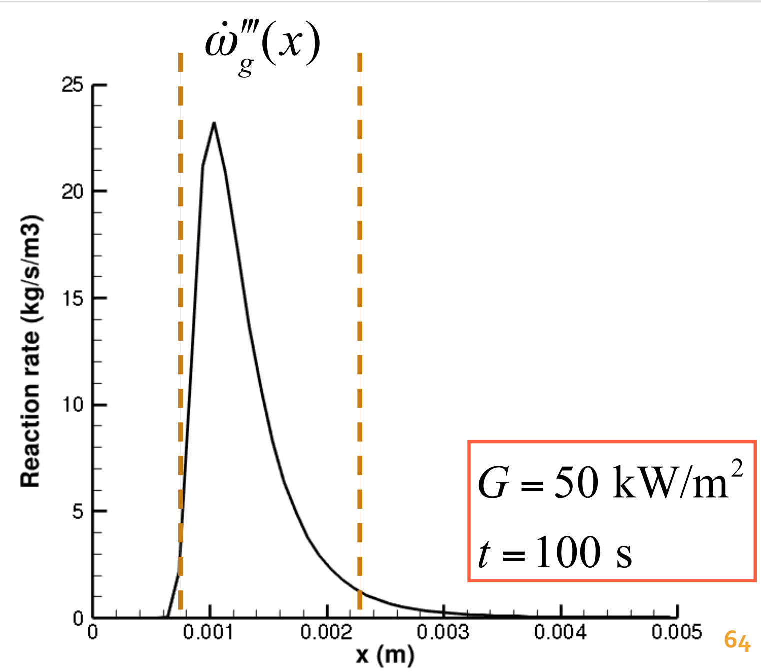


Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Example: PVC (Ghorbani & Trouvé, model from Stoliarov)

Instantaneous spatial variations inside PVC sample





Multi-Physics Modeling

- **Fuel source** modeling
  - Description of the fuel mass loss rate (MLR)
    - Finite-rate pyrolysis chemistry model: explicit treatment of thermal decomposition chemistry
    - Unknown model parameters:
      $(k,\rho,c,\varepsilon)_{vs},(k,\rho,c,\varepsilon)_{c},\eta_c,A,\ E,\ \Delta H_v$
    - Model parameters determined by comparison between model predictions and experimental results from micro-scale tests (*e.g*. thermogravimetric analysis) and material-scale tests (*e.g*. cone calorimeter, fire propagation apparatus)


6mm thick sample of PVC

Multi-Physics Modeling

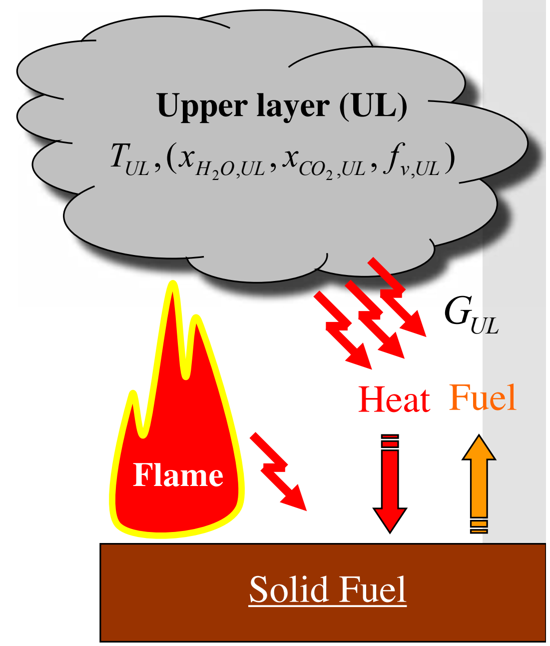
- **Soot** modeling
  - Motivation: soot contributes to, and often dominates thermal radiation transport in fires

$$\underbrace{G_{UL}}_{\text{emissive power}} = \underbrace{\varepsilon_{UL}}_{\text{emissivity}} \sigma T_{UL}^4$$

$$\underbrace{\varepsilon_{UL}}_{\text{emissivity}} = (1 - \exp(- \underbrace{\kappa_{UL}}_{\text{Planck mean absorption coef}} \times \underbrace{d_{UL}}_{\text{mean beam length}}))$$

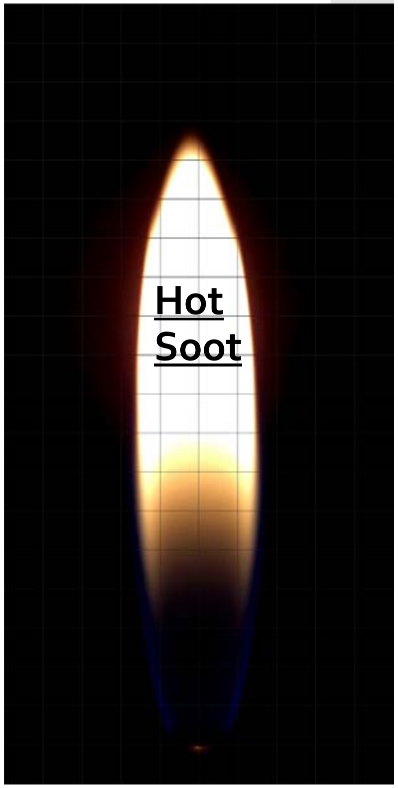
$$\underbrace{\kappa_{UL}}_{\text{Planck mean absorption coef}} = \underbrace{p(x_{H_2O,UL} a_{H_2O}(T) + x_{CO_2,UL} a_{CO_2}(T))}_{\text{gas component}} + \underbrace{C_{soot} f_{v,UL} T_{UL}}_{\text{soot component}}$$

often dominant



Multi-Physics Modeling

- **Soot** modeling
  - Motivation: thermal radiation transport
    - 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)



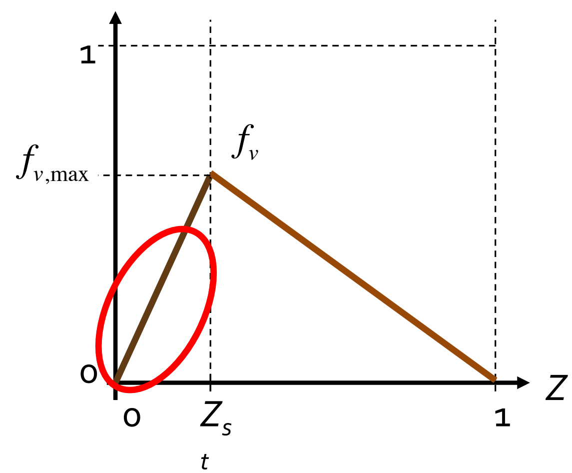
Multi-Physics Modeling

- **Soot** modeling
  - Soot yield model

$$C_nH_mO_p + \{n + (m/4) - (p/2) - (\nu_{CO}/2) - \nu_{soot}\}O_2$$
$$\rightarrow (n - \nu_{CO} - \nu_{soot})CO_2 + (m/2)H_2O + \underbrace{\nu_{CO}CO}_{\text{carbon monoxide}} + \underbrace{\nu_{soot}C}_{\text{soot}}$$

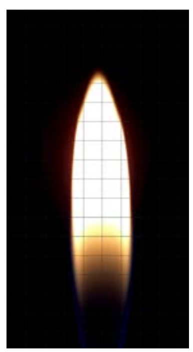
$$\eta_{soot} = \frac{\nu_{soot} \times W_{soot}}{W_{C_nH_mO_p}}$$

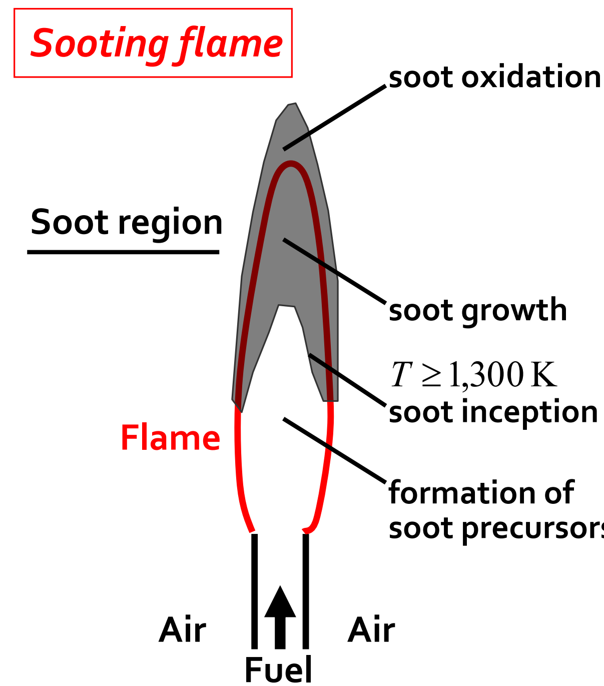
$$\overline{f_v} = \left(\frac{\bar{\rho}}{\rho_s}\right)\left(\frac{\eta_{soot}}{\eta_{CO_2}}\right)\tilde{Y}_{CO_2}$$



Multi-Physics Modeling

- **Soot** modeling
  - Description of soot formation/oxidation
    - 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





Multi-Physics Modeling

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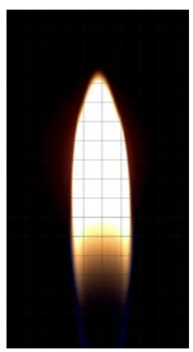
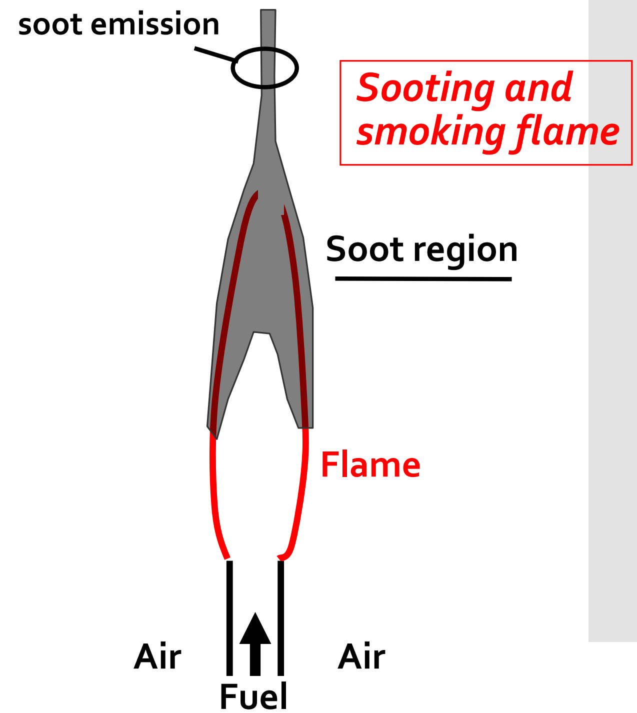




Multi-Physics Modeling

- **Soot** modeling
  - Laminar smoke point
    - A useful measure of a fuel tendency to form soot (sooting tendency is inversely proportional to smoke point)
    - Typical values of SP
      - ✓ Methane: infinity
      - ✓ Ethane: 0.24 m
      - ✓ Ethanol: 0.227 m
      - ✓ Polymethylmethacrylate (PMMA): 0.105 m
      - ✓ Ethylene: 0.097 m
      - ✓ Polypropylene (PP): 0.05 m
      - ✓ Polystyrene (PS): 0.015 m

Multi-Physics Modeling

- **Soot** modeling
  - One-equation model

$$\frac{\partial}{\partial t}(\rho_s \overline{f_v}) + \frac{\partial}{\partial x_i}(\rho_s \overline{f_v}\tilde{u}_i) = -\frac{\partial}{\partial x_i}(\rho_s \overline{f_v}\tilde{V}_{t,i}) + \frac{\partial}{\partial x_j}(\frac{\rho_s}{\overline{\rho}}\frac{\mu_t}{Sc_t}\frac{\partial \overline{f_v}}{\partial x_j}) + \overline{\dot{\omega}}_s'''$$

    - Thermophoretic transport
      - ✓ Small particles in a temperature gradient are driven from high to low temperature regions; free-molecular regime ($Kn = (2\lambda/d) >> 1$; $\lambda = 65$ nm)

$$V_{t,i} \approx -0.54\nu \frac{1}{T}\frac{\partial T}{\partial x_i}$$

    - Model parameters for $\overline{\dot{\omega}}_s'''$ are designed to be multi-fuel-compliant using an assumed correlation with laminar smoke point (SP) measurements (Delichatsios, *Combust. Sci. Technol*. 1994, Lautenberger, de Ris, Dembsey, Barnett & Baum, *Fire Safety J*. 2005)

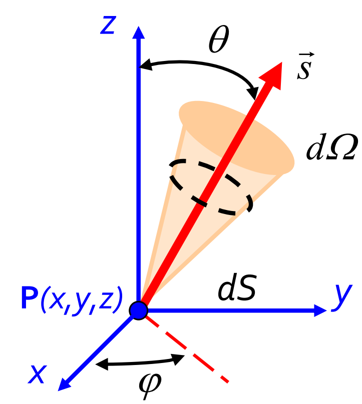
Multi-Physics Modeling

- **Radiation** modeling
  - Motivation: radiation transport generally dominates the gas-to-fuel-source thermal feedback
    - Radiation transport calculated via solving the radiative transfer equation
    - Assumptions
      - ✓Non-scattering medium
      - ✓Spectrally-averaged (grey medium) or spectrally-resolved radiation properties
      - ✓Planck mean absorption coefficient function of CO_2, H_2O and soot

Multi-Physics Modeling

- **Radiation** modeling
  - Radiative transfer equation (RTE)

$$\frac{dI}{ds}(P,\vec{s}) = \underbrace{\kappa\left(\frac{\sigma T^4}{\pi}\right)}_{\text{Emission}} - \underbrace{\kappa I(P,\vec{s})}_{\text{Absorption}} - \underbrace{\sigma_s I(P,\vec{s})}_{\text{Out-scattering}} + \underbrace{\sigma_s \int_{4\pi\ \text{sr}} I(P,\vec{i})\frac{\Phi(\vec{i}\rightarrow\vec{s})}{4\pi}d\Omega}_{\text{In-scattering}}$$



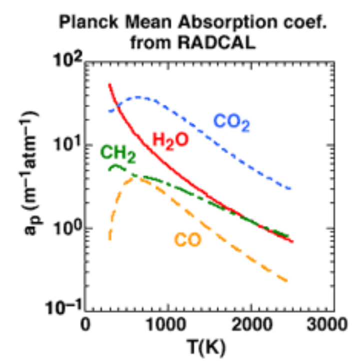
Multi-Physics Modeling

- **Radiation** modeling
  - Radiative transfer equation (RTE): without scattering

$$\frac{dI}{ds}(P,\vec{s}) = \underbrace{\kappa(\frac{\sigma T^4}{\pi})}_{\text{Emission}} - \underbrace{\kappa I(P,\vec{s})}_{\text{Absorption}}$$

- 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}]. $a_{p,i}$ is a function of temperature and is obtained from databases for radiative properties.

✓ κ_{soot} is the soot mean absorption coefficient [m^{-1}]

$$\kappa_{soot} = C_{soot} \times \boxed{f_v} T$$

Multi-Physics Modeling

- **Radiation** modeling
  - Solution methods for the radiative transfer equation (RTE)
    - **Discrete Transfer Method** (DTM, Lockwood & Shah, *Proc. Comb. Inst.*, 1981): a ray-tracing approach in which the RTE is solved along a set of representative rays
    - **Discrete Ordinate Method** (DOM, Chandrasekhar, *Radiative Transfer*, Dover, 1950): an Eulerian-grid-based approach in which the RTE is solved for a set of elementary angular regions
    - **Monte Carlo Method** (MCM): a Lagrangian particulate approach in which the RTE is replaced by a set of probabilistic rules that describe the transport of photons

Multi-Physics Modeling

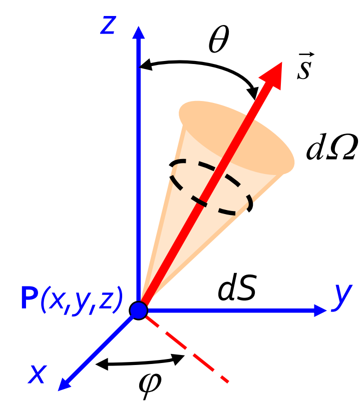
- **Radiation** modeling
  - Solution methods for the radiative transfer equation (RTE)
    - High computational cost (typically multiplies the cost of CFD by a factor of at least 2)
    - An elliptic problem that usually requires an iterative solution

Multi-Physics Modeling

- **Radiation** modeling
  - Radiative transfer equation (RTE)
    - Radiative heating/cooling rate (in gas energy equation) [W/m3]

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

$$\dot{q}'''_{rad} = -\int_{4\pi\ \mathrm{sr}} \frac{dI}{ds} d\Omega = -4\kappa(\sigma T^4) + \int_{4\pi\ \mathrm{sr}} \kappa I \, d\Omega$$



Multi-Physics Modeling

- **Radiation** modeling
  - Radiative transfer equation (RTE)
    - LES framework

$$\nabla \bar{I}.\vec{s} = \underbrace{\overline{\kappa\left(\frac{\sigma T^4}{\pi}\right)}}_{\substack{\text{Emission} \\ \text{(grid-resolved and} \\ \text{subgrid-scale)}}} - \underbrace{\overline{\kappa I}}_{\substack{\text{Absorption} \\ \text{(grid-scale and} \\ \text{subgrid-scale)}}}$$

requires modeling

$$\boxed{\overline{\dot{q}'''_{rad}} = -4\overline{\kappa(\sigma T^4)} + \int_{4\pi \text{ sr}} \overline{\kappa I}\, d\Omega}$$

Multi-Physics Modeling

- **Radiation** modeling
  - Radiative transfer equation (RTE)
    - Closure model for RTE (LES framework): the prescribed **radiant fraction** approach

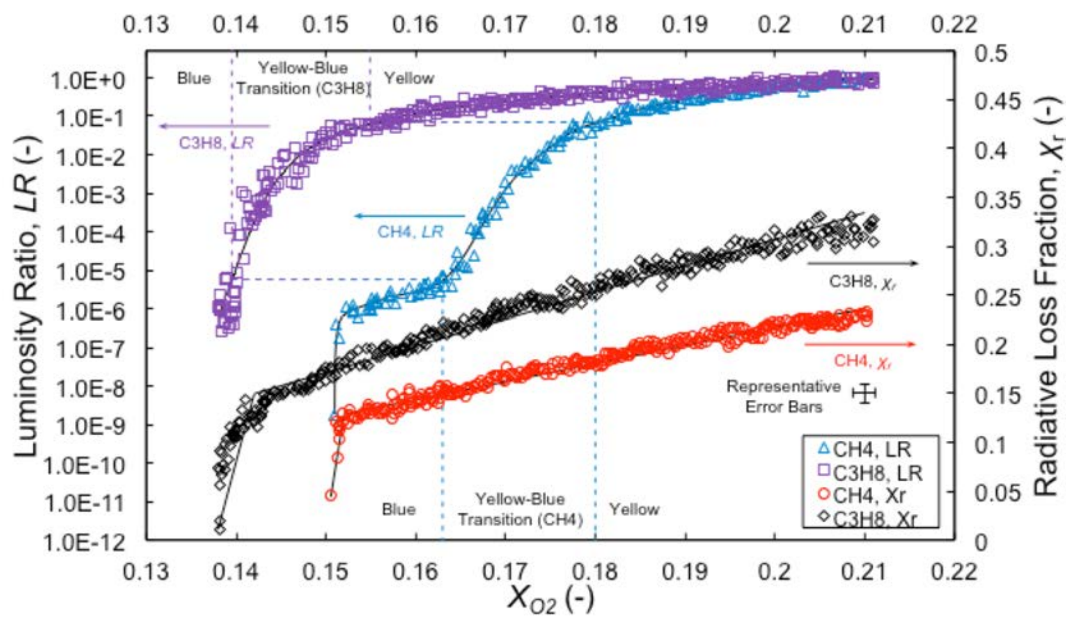
$$\nabla \bar{I}.\vec{s} = \chi_{rad} \times \left(\frac{\dot{q}'''_{comb}}{4\pi}\right), \quad \text{if } \dot{q}'''_{comb} > 0$$

$$\nabla \bar{I}.\vec{s} = 0, \ \text{if } \dot{q}'''_{comb} = 0$$

    - Radiant fraction χ_{rad} is treated as an input quantity to the fire model and is user-prescribed

Multi-Physics Modeling

- **Radiation** modeling
  - Radiant fraction χ_{rad} is generally an input quantity



White, Link, Trouvé, Sunderland, Marshall, Sheffel, Corn, Colket, Chaos & Yu, *Fire Safety J.*, 2015

State of the Art

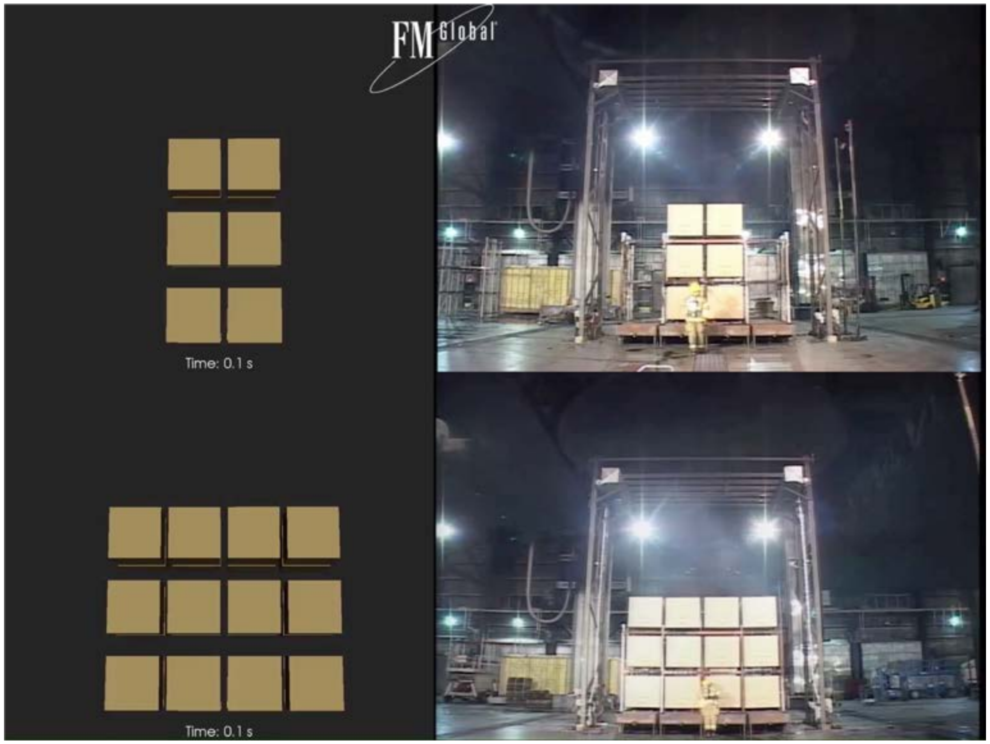
- **Examples**

	FireFOAM[1]	FDS[2]
Scheme	Second-order accurate, finite volume solver with implicit time integration	Second-order accurate, finite difference solver with explicit time integration
Turbulence	*k*-eqn model (default), dynamic Smagorinsky, WALE, Deardorff	Deardorff (default), dynamic Smagorinsky
Combustion	Global combustion eqn, Eddy Dissipation Concept (EDC)	Global combustion eqn, Eddy Dissipation Concept (EDC)
Radiation	Finite volume method (prescribed radiant fraction, grey medium model or a spectrally-resolved wide band model)	Finite volume method (prescribed radiant fraction, grey medium model or a spectrally-resolved wide band model
Soot	Flamelet-based model	Soot yield model
Mesh	Structured and unstructured grid	Structured (Cartesian) grid

[1] FM Global (USA), FireFOAM, Available from: https://github.com/fireFoam-dev/fireFoam-2.2.x
[2] NIST (USA), FDS, Available from: https://code.google.com/p/fds-smv/

State of the Art

- **Example:** Coarse-grained LES (engineering-level) (FireFOAM)
  - FM Global full-scale flame spread tests
  - Flame structure: L ~ O(10 m); L_{eddy} ~ O(10 cm); U_{eddy} ~ O(1-10 m/s)



(Wang, Meredith, Zhou, Chatterjee, Xin, Chaos, Ren & Dorofeev, *Proc. 11th Intl. Symp. Fire Safety Science*, IAFSS, 2014)

State of the Art

- **Example:** Coarse-grained LES (engineering-level) (FDS)
  - UMD side-by-side burn test
  - Flame structure: L ~ O(1 m); L_{eddy} ~ O(10 cm); U_{eddy} ~ O(1 m/s)

(Gardner, Horst, Pfarr, Scott, Steranka, West, Wood, Zeller, Isman, Trouvé, UMD, 2018)

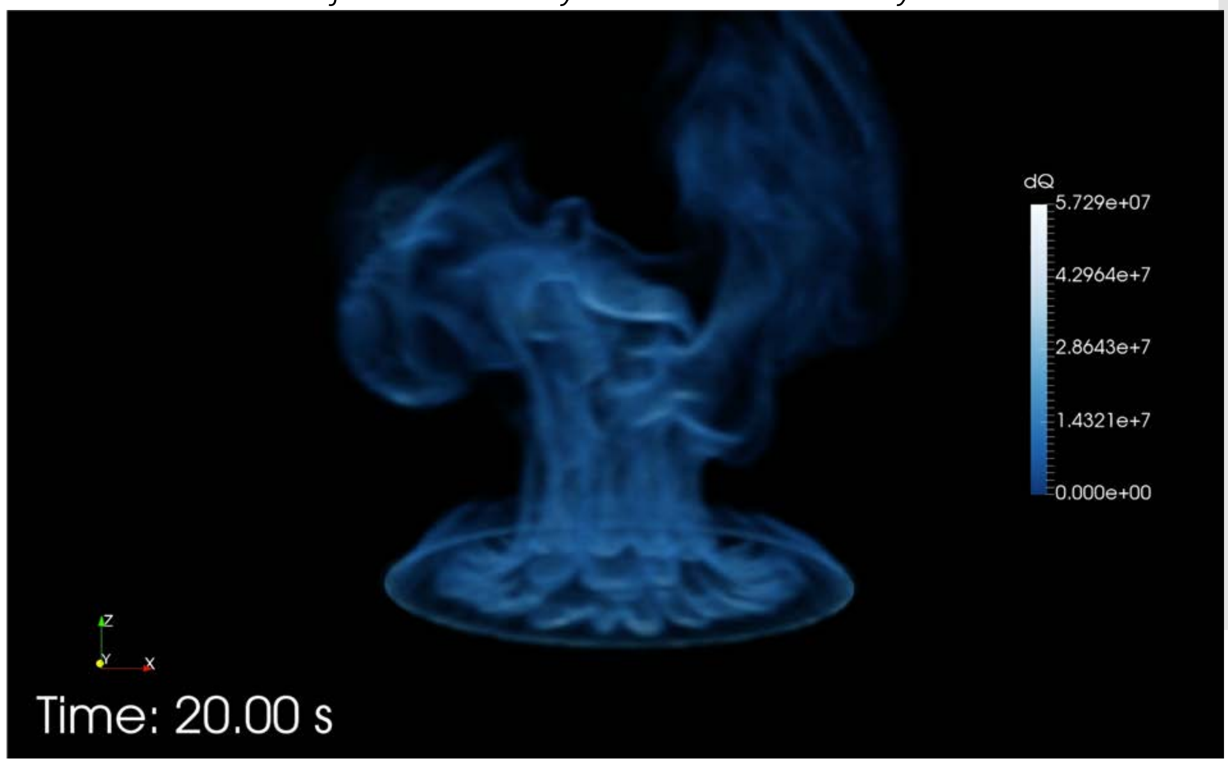
State of the Art

- **Example:** Fine-grained LES (research-level) (FireFOAM)
  - UMD experiment on flame suppression by inert gas or water mist
  - Flame structure: L_f ~ 0.5 m; L_{eddy} ~ O(1-10 cm); U_{eddy} ~ O(1 m/s)

(Vilfayeau, White, Sunderland, Marshall, Trouvé, *Fire Safety J.*, 2016)

State of the Art

- **Example:** Fine-grained LES (research-level) (FireFOAM)
  - University of Waterloo experiment on methanol pool fire
  - Flame structure: L_f ~ 0.5 m; L_{eddy} ~ O(2-30 cm); U_{eddy} ~ O(1 m/s)



(Marchand, Verma, Trouvé, *unpublished.*, 2018)

Conclusion

- The fire modeling community has experienced a remarkable growth in the past two decades
  - Due in particular to the development of FDS (NIST) and FireFOAM (FM Global) as well as to the development of open-source CFD software
- Fire modeling features several technical challenges
  - Relatively slow, buoyancy-driven flow
  - Boundary layer flames
  - Flame extinction/ignition
  - Modeling of solid fuel sources (pyrolysis processes)
  - Soot formation
  - Spectrally-resolved radiation and radiation-turbulence interactions
  - Water spray
  - Flame and smoke chemistry effects (toxicity)

Conclusion

- The fire modeling community faces an organizational challenge
  - The fire modeling community is small, fragmented, geographically dispersed, without a history of well-defined standards and without a consensus on well-defined objectives
  - There is a need for a coordinated effort to organize and strengthen the fire modeling community
- MaCFP
  - The IAFSS Working Group on Measurement and Computation of Fire Phenomena (*http://www.iafss.org/macfp/*)
    - A forum between experimentalists and modelers to establish a common framework around the topic of CFD validation
    - A regular series of workshops
    - A list of community-approved target experiments
    - A data repository (*https://github.com/MaCFP*)