

Modeling Tasks for the 3rd International Workshop on Laser-Induced Incandescence

- File format:** ASCII, 49 columns, space delimited
first column: time base
other columns: defined by Cases 1-8 given below
Case 9 give in separate block
Case 10 give in header for D_{ave} or separate block for distribution
- Timescale:** Run out to at least 500 ns with a time resolution of your choice
- Laser:** wavelength: 1064 nm
temporal profile: see attached file
spatial profile: tophat, i.e., single fluence
- Detection:** wavelength: 680 nm square bandpass
time resolution: infinitely fast
- Signal collection:** don't include corrections for the solid angle element and detector quantum efficiency.
- Primary particles:** diameter: 35 nm, monodisperse

Numbers and descriptions of simulation cases:

Melton Model with fixed parameters (see next page):

Case 1: 1650 K, 1 bar, 0.1 J/cm²

Case 2: 1650 K, 1 bar, 0.8 J/cm²

Free model and free parameters:

Case 3: 1650 K, 1 bar, 0.1 J/cm²

Case 4: 1650 K, 1 bar, 0.8 J/cm²

Case 5: 300 K, 1 bar, 0.1 J/cm²

Case 6: 300 K, 1 bar, 0.8 J/cm²

Case 7: 1650 K, 10 bar, 0.1 J/cm²

Case 8: 1650 K, 10 bar, 0.8 J/cm²

Case 9: 1650 K, 1 bar, Peak signal and peak temperature for fluences of 0.05, 0.10, 0.15, 0.20, 0.25, 0.30, 0.35, 0.40, 0.50, 0.60, 0.80, 1.00, and 1.5 J/cm²

Case 10: evaluate average diameter or polydisperse distribution from LII signal in attached file at 1650 K, 1 bar, 0.1 J/cm², detection wavelength 680 nm

For Cases 1 and 2 include calculated values for

- a: Particle temperature
- b: Particle diameter
- c: LII signal

For Cases 3-8 include calculated values for

- a: Particle temperature
- b: Particle diameter
- c: LII signal
- d: $Q_{\text{absorption}}$
- e: $Q_{\text{conduction}}$
- f: $Q_{\text{radiation}}$
- g: $Q_{\text{sublimation}}$

Submission of the results: Please email to Hope (hamiche@sandia.gov), and/or Fengshan (Fengshan.Liu@nrc-cnrc.gc.ca), and/or Henrik (henrik.bladh@forbrf.lth.se).

Melton Model with Fixed Parameters

Energy conservation equation:

$$\frac{\pi^2 D^3 E(m)}{\lambda_l} F q(t) - \frac{2\kappa_a \pi D^2}{(D + GL)} (T - T_g) + \frac{\Delta H_v}{W_v} \frac{dM}{dt} - \frac{\pi D^3 \rho_s c_s}{6} \frac{dT}{dt} = 0 \quad (1)$$

D : Particle diameter = 35×10^{-7} cm

λ_l : Laser wavelength = 1064×10^{-7} cm

$E(m)$: Wavelength dependent function of the soot refractive index = 0.23

F : Laser fluence in J/cm^2

$q(t)$: Laser temporal power density per unit laser fluence = $q(\text{supplied})/q_0$ 1/s

q_0 : Normalization for laser temporal profile = 1.16278×10^{-8}

κ_a : Thermal conductivity of air at 1650 K and 1 bar = 9.6×10^{-4} J/(cm s K)

T : Particle temperature in K

T_g : Gas (also particle initial) temperature = 1650 K

L : Mean free path of air at 1 bar = $2.355 \times 10^{-8} \times T_g$ cm

G : Geometry-dependent heat transfer factor = $8f/[\alpha(\gamma+1)]$

f : Eucken factor = $(9\gamma-5)/4$

α : Thermal accommodation coefficient = 0.3

γ : Specific heat ratio of air at 1650 K = 1.3

ΔH_v : Heat of sublimation of carbon = 7.78×10^5 J/mol

W_v : Molecular weight of sublimed carbon assuming C_3 only sublimes = 36 g/mol

M : Mass of the particle in g

t : Time in s

ρ_s : Density of carbon = 2.26 g/cm³

c_s : Specific heat of carbon = 1.90 J/(g K)

Mass conservation equation:

$$\frac{dM}{dt} = \frac{-\pi D^2 W_v p_v}{R_p T} \left(\frac{R_m T}{2W_v} \right)^{0.5} \quad (2)$$

p_v : Vapor pressure in bar = $p_{ref} \exp[\Delta H_v(T - T_{ref})/(RTT_{ref})]$

p_{ref} : = 1 bar

T_{ref} : = 3915 K

W_v : Molecular weight of carbon vapour = 36 g/mol

R : Universal gas constant = 8.31 J/(K mol)

R_m : Universal gas constant = 8.31×10^7 g cm²/(K mol s²)

R_p : Universal gas constant = 83.1 bar cm³/(K mol)

Signal calculation:

$$S = \frac{8\pi^3 D^3 h c^2 E(m)}{\lambda_s^6 [\exp(hc/\lambda_s k_B T) - 1]} \quad (3)$$

h : Planck constant = 6.626×10^{-34} J s

c : Speed of light = 3.00×10^{10} cm/s

k_B : Boltzmann constant = 1.381×10^{-23} J/K

λ_s : Emission wavelength = 680×10^{-7} cm for this comparison