

Turbulent Combustion Rates in Aluminum-air Clouds at Different Scales

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1 Introduction

In the past, we have studied turbulent combustion effects in both confined [1,2] and unconfined [3] explosions. And we have proposed *gasdynamic models* [4] and *heterogeneous continuum models* [5] for the turbulent combustion fields. More recently we have proposed an *induction-time model* [6] for the ignition of Al particle clouds. It is based on Arrhenius fits to the shock tube data of Boiko [7,8]. This paper explores “scaling issues” associated with Al particle combustion in explosions. The research idea is the following:

- This is a non-premixed combustion system; the global burning rate is controlled by rate of turbulent mixing of fuel (Al particles) with air. For similitude reasons, the turbulent mixing rates should scale with the explosion length and time scales, i.e., $r(cm/g^{1/3})$ and $t(ms/g^{1/3})$.
- However, the induction time [6] for ignition of Al particles depends on the *Arrhenius Function*: $t_1 = 2.5 \times 10^{-8} e^{30,000/T}$, which is independent of the explosion length and time scales.

To study this, we have performed numerical simulations of turbulent combustion in unconfined Al-SDF (shock-dispersed-fuel) explosion fields at different scales. Three different charge masses were assumed: 1-g, 1-kg and 1-T Al-powder charges. We found that there are two combustion regimes: an *ignition regime*—where the burning rate decays a power law function of time, and a *turbulent combustion regime*—where the burning rate decays as an exponentially with time. The **Model**, including the conservation laws with interphase interactions, combustion and ignition models, equations of state and numerical methods are described in §2. This is followed by **Results** and **Conclusions** in §3 and §4.

2 Model

Conservation Laws

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The Model is based on the Eulerian multi-phase conservation laws for a dilute heterogeneous continuum, as formulated by Nigmatulin [9]. We model the evolution of the gas phase combustion fields in the limit of large Reynolds and Peclet numbers, where effects of molecular diffusion and heat conduction are negligible. The flow field is governed by the gas-dynamic conservation laws:

$$\text{Mass:} \quad \partial_t \rho + \nabla \cdot (\rho \mathbf{u}) = \dot{\sigma}_s \quad (1)$$

$$\text{Momentum:} \quad \partial_t \rho \mathbf{u} + \nabla \cdot (\rho \mathbf{u} \mathbf{u} + p) = \dot{\sigma}_s \mathbf{v} - \dot{f}_s \quad (2)$$

$$\text{Energy:} \quad \partial_t \rho E + \nabla \cdot (\rho \mathbf{u} E + p \mathbf{u}) = -\dot{q}_s + \dot{\sigma}_s E_s - \dot{f}_s \cdot \mathbf{v} \quad (3)$$

where ρ, p, U represent the gas density, pressure and specific internal energy, $\mathbf{u}$ is the gas velocity vector, and $E = U + \mathbf{u} \cdot \mathbf{u} / 2$ denotes the total energy of the gas phase. Source terms on the right hand side take into account: mass addition to gas phase due to particle burning ($\dot{\sigma}_s$), particle drag ($\dot{f}_s$), and heat losses ($\dot{q}_s$).

We treat the particle phase as a Eulerian continuum field [9]. We consider the dilute limit, devoid of particle-particle interactions, so that the pressure and sound speed of the particle phase are zero. We model the evolution of particle phase mass, momentum and energy fields by the conservation laws of continuum mechanics for heterogeneous media:

$$\text{Mass:} \quad \partial_t \sigma + \nabla \cdot (\sigma \mathbf{v}) = -\dot{\sigma}_s \quad (4)$$

$$\text{Momentum:} \quad \partial_t \sigma \mathbf{v} + \nabla \cdot (\sigma \mathbf{v} \mathbf{v}) = -\dot{\sigma}_s \mathbf{v} + \dot{f}_s \quad (5)$$

$$\text{Energy:} \quad \partial_t \sigma E_s + \nabla \cdot (\sigma E_s \mathbf{v}) = \dot{q}_s - \dot{\sigma}_s E_s + \dot{f}_s \cdot \mathbf{v} \quad (6)$$

where σ and $\mathbf{v}$ represent the particle-phase density and velocity, and $E_s = C_s T_s + \mathbf{v} \cdot \mathbf{v} / 2$ denotes the total energy of the particle phase.

Interactions

The inter-phase interaction terms for mass, momentum, heat and particle burning law take the form as described by Veyssiere and Khasainov [10]:

$$\text{Mass Exchange:} \quad \dot{\sigma}_s = \begin{cases} 0 & f < 1 \\ \dot{\sigma}_2 & f = 1 \end{cases} \quad (7)$$

$$\text{Momentum Exchange:} \quad \dot{f}_s = (3r_s / 4r_s d_s) C_D (\mathbf{u} - \mathbf{v}) |\mathbf{u} - \mathbf{v}| \quad (8)$$

$$\text{Drag Coefficient:} \quad C_D = 24 / \text{Re}_s + 4.4 / \sqrt{\text{Re}_s} + 0.42 \text{ and } \text{Re}_s = r_s |\mathbf{u} - \mathbf{v}| / \eta \quad (9)$$

$$\text{Heat Exchange:} \quad \dot{q}_s = (6s / r_s d_s) \left[Nu / (T - T_s) / d_s + \epsilon_{\text{Boltz}} (T^4 - T_s^4) \right] \quad (10)$$

$$\text{Convective Heat Transfer:} \quad Nu = 2 + 0.6 \text{Pr} \sqrt{\text{Re}_s} \quad (11)$$

Combustion

We consider two fuels: PETN detonation products (F_1) from the booster, and Aluminum (F_2), along with their corresponding combustion products: PETN-air (P_1) and Al-air (P_2). We model the global combustion of the fuels F_k with air (A) producing equilibrium combustion products P_k :

$$F_k + A_k \rightarrow P_k \quad (k = 1, 2) \quad (12)$$

The mass fractions Y_k of the components are governed by component conservation laws; in the limit of large Peclet numbers (where molecular diffusion effects are negligible) they become:

$$\text{Fuel-}k: \quad \nabla \cdot (r Y_{Fk} \mathbf{u}) = -\dot{s}_k \quad (13)$$

$$\text{Air:} \quad \nabla \cdot (r Y_{Ak} \mathbf{u}) = -\sum_k a_k \dot{s}_k \quad (14)$$

$$\text{Products-}k: \quad \nabla \cdot (r Y_{Pk} \mathbf{u}) = \sum_k (1 + a_k) \dot{s}_k \quad (15)$$

Fuel and air are consumed in stoichiometric proportions: $\dot{a}_k = A_k / F_k$. In the above, $\dot{s}_k$ represents the global kinetics term. For PETN-air combustion, we assume combustion is mixing limited, so we use

the fast-chemistry approximation: whenever fuel and air enter a computational cell, they are consumed in one time step. For Al-air combustion, we use an induction-time model described below.

Ignition

Following Korobeinikov et al [11] and Oran et al [12] for premixed systems, we define an induction-time fraction: $f(\mathbf{x}, t)$, which is initialized to zero: $f(\mathbf{x}, 0) = 0$ and grows to 1 at the end of the ignition delay. It evolves according to the following advection equation:

$$\text{Induction Model:} \quad \mathcal{L}f + \mathbf{v} \cdot \nabla f = f / t_i \quad (16)$$

The induction time, t_i , is based on an Arrhenius fit to Boiko's Al particle data [7,8]:

$$\text{Induction Time:} \quad t_i = A e^{E_0/RT} \quad (17)$$

Figure 1 presents data and fits for three particle compositions: data 1: 3-5 μm Al spheres; data 2: 0-20 μm Al-Fe spheres; and data 3: Al flakes, 20-30 μm x 2-5 μm thickness. The slope represents the activation energy which is 30 kCal for Al particles and 34 k-Cal for Al-Fe spheres. Note that this data is in the "normal" self-ignition regime ($T \sim 1,800$ K)¹.

Figure 2 presents streak photography records for shock-induced ignition of Al particle clouds. Three fuel loadings were used: (a) 5 mg, (b) 1 mg and (c) 0.25 mg. One can see that in cases (a) and (b) the entire cloud ignited, while in case (c) a few particles ignited but then burned out—so the entire cloud was not ignited. We call this "multi-particle effects" on cloud ignition, and represent it mathematically as an ignition probability model [6]:

$$\text{Ignition Probability:} \quad \eta(s) = \frac{1}{1 + \exp[(s_0 - s)/b]} \quad (18)$$

shown in Fig. 3. Here s_0 denotes the value of particle concentration resulting in a 50 % probability of cloud ignition, while b represents the slope parameter which determines the width of the probability function. For ignition of flake Al particles in air, they acquire the following values: $s_0 = 130 \text{ g/m}^3$ and $b = 20$. Equation (18) was determined empirically by fitting data from the Al particle cloud experiments of Boiko [7,8]. It models the requirement that the **local** concentration of particles must be large enough so that ignition of one particle can be passed on to its neighbors—a cloud ignition effect—in contrast to the single-particle ignition effect. Being based on experimental data, it implicitly presumes that the local mixture is within the flammability limits of the Al-air system considered. Finally, ignition occurs when $f = 1$; then the source term becomes:

$$\text{Ignition:} \quad \dot{s}_2 = \dot{s}_s \times \eta(s) \quad (19)$$

Equations of State

The thermodynamic states encountered during SDF explosions have been analyzed in by Kuhl and Khasainov [13]. The locus of states of component c in specific internal energy-temperature plane are fit with quadratic functions of temperature:

$$U_c = a_c T^2 + b_c T + c_c \quad (20)$$

For cells containing a mixture of components, the mixture energy also satisfies a quadratic form:

¹ We note in passing, that Boiko [7,8] also found "irregular" ignition regimes: one grouped near $T \sim 1,250$ K and one grouped near $T \sim 950$ K. Such regimes depend on other mechano-chemical effects (oxide coating, cracks, etc.) thereby complicating the problem. For simplicity we only study the normal ignition regime.

$$U_m(T) = \sum_c \dot{a}_c Y_c U_c = a_m T^2 + b_m T + c_m \quad (21)$$

Given the mixture specific internal energy U_m the mixture temperature can be evaluated by:

$$T_m = [-b_m + \sqrt{b_m^2 - 4a_m(c_m - U_m)}] / 2a_m \quad (22)$$

using mixture coefficients as defined by:

$$a_m = \sum_c \dot{a}_c Y_c a_c, \quad b_m = \sum_c \dot{a}_c Y_c b_c, \quad c_m = \sum_c \dot{a}_c Y_c c_c, \quad R_m = \sum_c \dot{a}_c Y_c R_c \quad (23)$$

For pure cells, the pressure of a component is calculated from the perfect gas relation $p_c = r_c R_c T_c$, or from the JWL function in the detonation products gases [13]. In mixed cells, the pressure is calculated from the mixture temperature by the “law of additive pressures”: $p_m = \sum_c \dot{a}_c p_c(V_m, T_m)$ where $p_c(V_m, T_m)$ denotes the pressure of component c if it existed alone at V_m and T_m .

Numerical Methods

The governing equations (1)-(6) and (13)-(15) were integrated with high-resolution upwind methods that represent high-order generalizations of Godunov’s method. The algorithm for gas phase conservation laws is based on an efficient Riemann solver for gas-dynamics first developed by Colella and Glaz [14]. The algorithm for the particle phase conservation laws is based on a Riemann solver for two-phase flows as developed by Collins et al. [15]. Source terms are treated with operator splitting methods. Being based on Riemann solvers, information propagates along characteristics at the correct wave speeds, and they incorporate nonlinear wave interactions within the cell during the time step.

These Godunov schemes have been incorporated into an adaptive mesh refinement (AMR) algorithm of Berger & Colella [16] that allows us to focus computational effort in complex regions of the flow such as mixing layers and reaction zones. In this AMR approach, regions to be refined are organized into rectangular patches, with hundreds to thousands of grid-points per patch. AMR is also used to refine turbulent mixing regions; by successive refinements we are able to capture the energy-bearing scales of the turbulence on the computational grid. In this way we are able to compute the effects of turbulent mixing without resorting to turbulence modeling (which is not applicable to this problem). This is consistent with the “MILES” approach of Boris et al. [17].

3 Results

Initial Conditions

We studied blast waves from spherical Shock-Dispersed-Fuel (SDF) charges containing Aluminum powder: three different charge masses were assumed:

- Charge 1: 0.5-g spherical booster of PETN surrounded by 1-g shell of Aluminum powder
- Charge 2: 0.5-kg spherical booster of PETN surrounded by 1-kg shell of Aluminum powder
- Charge 3: 0.5-T spherical booster of PETN surrounded by 1-T shell of Aluminum powder

The charge was embedded in air at STP conditions. Detonation of the booster created a blast wave that dispersed the fuel, creating a two-phase combustion cloud.

Flow Visualization

Cross-sections of the fireball temperature fields are shown in Fig. 4 at the same scaled time of $t = 0.65 \text{ ms} / g^{1/3}$. At this time, the cloud diameters were: $d \sim 60\text{-cm}$, $d \sim 6\text{-m}$ and $d \sim 60\text{-m}$, respectively. While the cloud dimensions seem to cube-root scale, the domain of combustion (red regions) seems to be more extensive as the charge mass increases. This is born out in the fuel consumption discussed next.

Global Fuel Consumption

Mass-fractions of fuel consumed are presented in Fig. 5. We find two regimes:

$$\text{Ignition Regime:} \quad \dot{m}(t) \sim a \tau^{0.5} \quad \& \quad \dot{m} \sim 0.5a / \sqrt{t} \quad (24)$$

$$\text{Combustion Regime:} \quad \dot{m}(t) \sim 1 - a \times e^{-bt} \quad \& \quad \dot{m} \sim ab \times e^{-bt} \quad (25)$$

where $[t] = \text{ms} / g^{1/3}$. In the ignition regime, fuel consumption decays as $1/\sqrt{t}$, while in the combustion regime, fuel consumption decays exponentially with time. The first is controlled by the induction time model (equations 16 and 17), while the latter is a consequence of the turbulent combustion model. In *Appendix-A*, we show that global fuel consumption is proportional to fuel remaining, that is: $dm_F \propto -m_F$. This results in an exponential form for the fuel consumed: $\dot{m}(t) = 1 - e^{-t/\tau}$. This is a characteristic of first-order reactions as described by Kondratiev [18], and is a simplified form of the *Vibe Function* [19] that is used to represent combustion in engines [20], and the more general concept of *Life Functions* as described by Oppenheim and Kuhl [21], [22].

4 Conclusions

Numerical simulations were used to study turbulent combustion in fireballs created by the unconfined explosion of Al SDF charges. Three charge masses of Al powder were investigated: 1-g, 1-kg and 1-T. Fireball dimensions scaled as the cube root of the charge mass—illustrating that this is a gasdynamic effect. However, burning rates did not cube-root scale. At early times, the burning rate decayed as $1/\sqrt{t}$, while at later times the burning rate decayed exponentially with time: $e^{-t/\tau}$, where τ is the characteristic combustion time, which is controlled by the turbulent mixing rate. This exponential dependence is typical of first-order reactions, combustion cycles in engines and the more general concept of *Life Functions* that control the dynamics of evolutionary systems.

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Appendix A: Derivation of the Fuel Consumption Relation

Based on eq. (13), the fuel consumption model may be written as:

$$\nabla \cdot r_F \mathbf{u} = -\dot{s}_F \quad (\text{A1})$$

Combustion always occurs at the stoichiometric contour, so one can take

$$\dot{s}_F = r_F / t \quad (\text{A2})$$

where t represent the characteristic combustion time. Combining the above, one finds

$$\partial_t r_F + \nabla \cdot r_F \mathbf{u} = -r_F / t \quad (\text{A3})$$

Integrating over a spherical volume with of radius R gives:

$$\int_R \partial_t r_F dV + \int_R \nabla \cdot r_F \mathbf{u} dV = -\frac{1}{t} \int_R r_F dV \quad (\text{A4})$$

Taking the spherical radius to be larger than the shock front radius ($R > R_s$), flux through the outer boundary is zero (i.e., the second integral is zero), yielding:

$$\frac{d}{dt} m_F = -m_F / t \quad (\text{A5})$$

where $m_F = \int r_F dV$. Thus the fuel consumption equation becomes

$$\frac{d}{dt} \ln(m_F) = -1/t \quad (\text{A6})$$

Integrating (A6) yields:

$$\ln[m_F(t) / m_F(0)] = -t/t \quad (\text{A7})$$

Solving for the fuel mass fraction, one finds:

$$m_F(t) / m_F(0) = e^{-t/t} \quad (\text{A8})$$

Reverting the fuel consumed variable: $m(t) = 1 - m_F(t) / m_F(0)$, the above yields the exponential form:

$$m(t) = 1 - e^{-t/t} \quad (\text{A9})$$

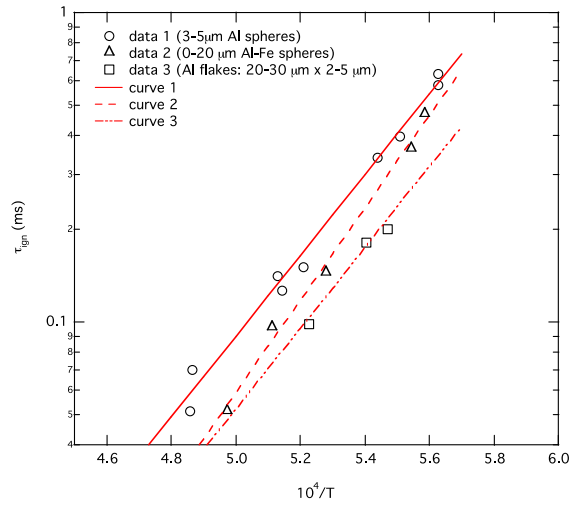


Figure 1. Measured ignition delays in the “normal ignition” regime ($T_* \sim 1,800\text{K}$) are plotted versus $1/T$ (Curve 1: $t_1 = 2.5 \cdot 10^{-8} e^{30,000/T}$; Curve 2: $t_2 = 0.2 \cdot 10^{-8} e^{34,400/T}$; Curve 3: $t_3 = 1.6 \cdot 10^{-8} e^{30,000/T}$).

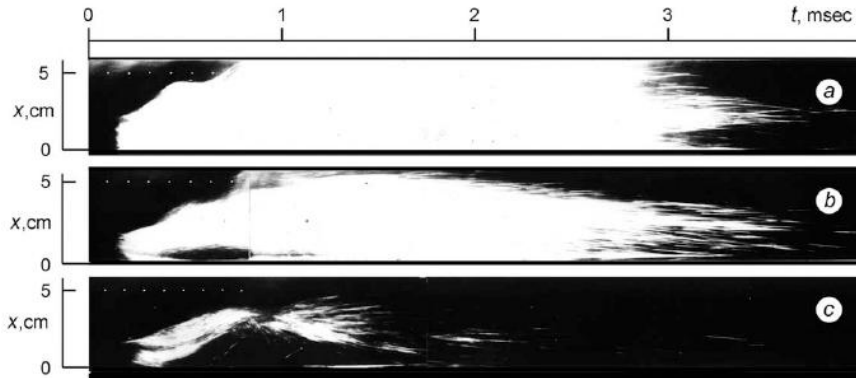


Figure 2. Streak photography of the ignition of an aluminum particle cloud at $T = 1900\text{ K}$ and $p = 1.1\text{ MPa}$ for different fuel loading, m : (a) $m = 5\text{ mg}$, (b) $m = 1\text{ mg}$, (c) $m = 0.25\text{ mg}$ (Boiko & Poplavski, 2002).

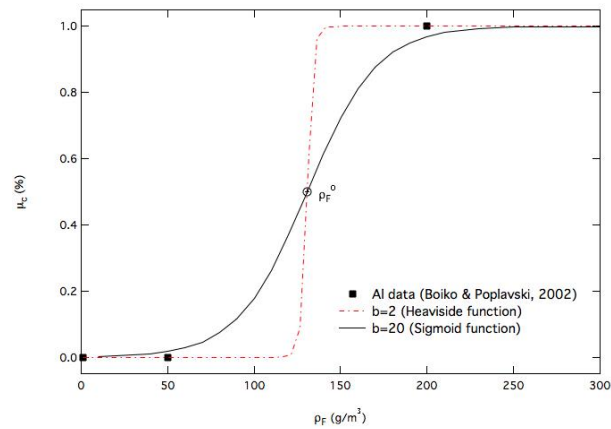


Figure 3. Ignition probability of a cloud of aluminum particles in the self-ignition regime ($T_* \sim 1,800\text{K}$) is plotted versus fuel loading: r_F , based on the shock tube experiments [7,8].

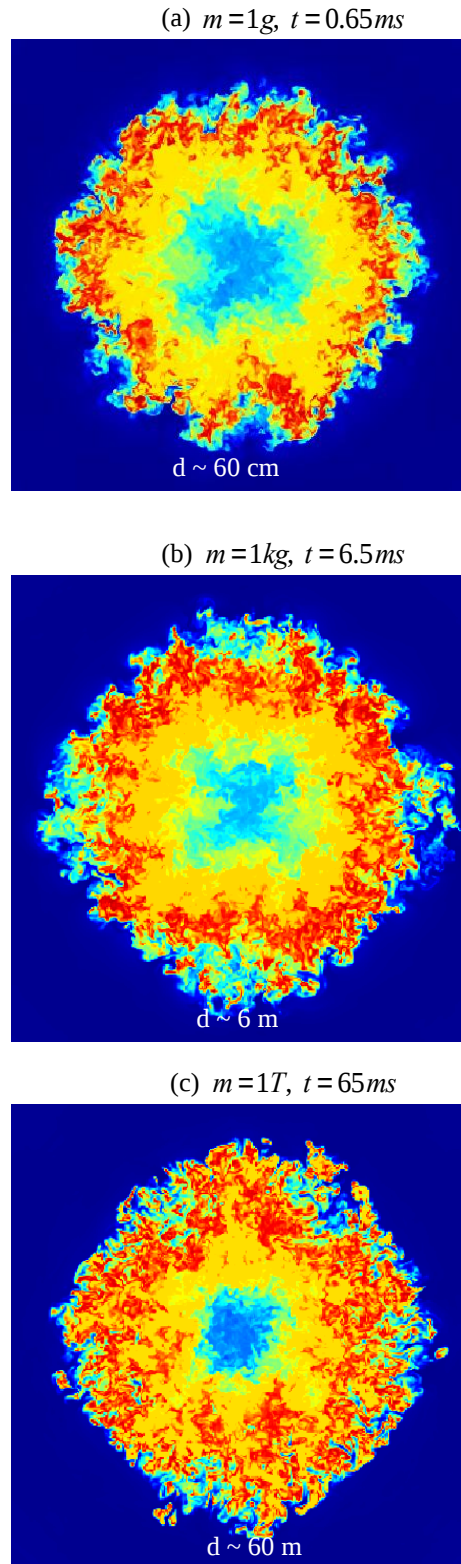


Figure 4. Cross-section of the computed fireballs showing the temperature fields at the same scaled time of $t = 0.65\text{ms} / g^{1/3}$; cloud dimensions are as follows: (a) $d \sim 60\text{ cm}$, (b) $d \sim 6\text{ m}$, (c) $d \sim 60\text{ m}$.

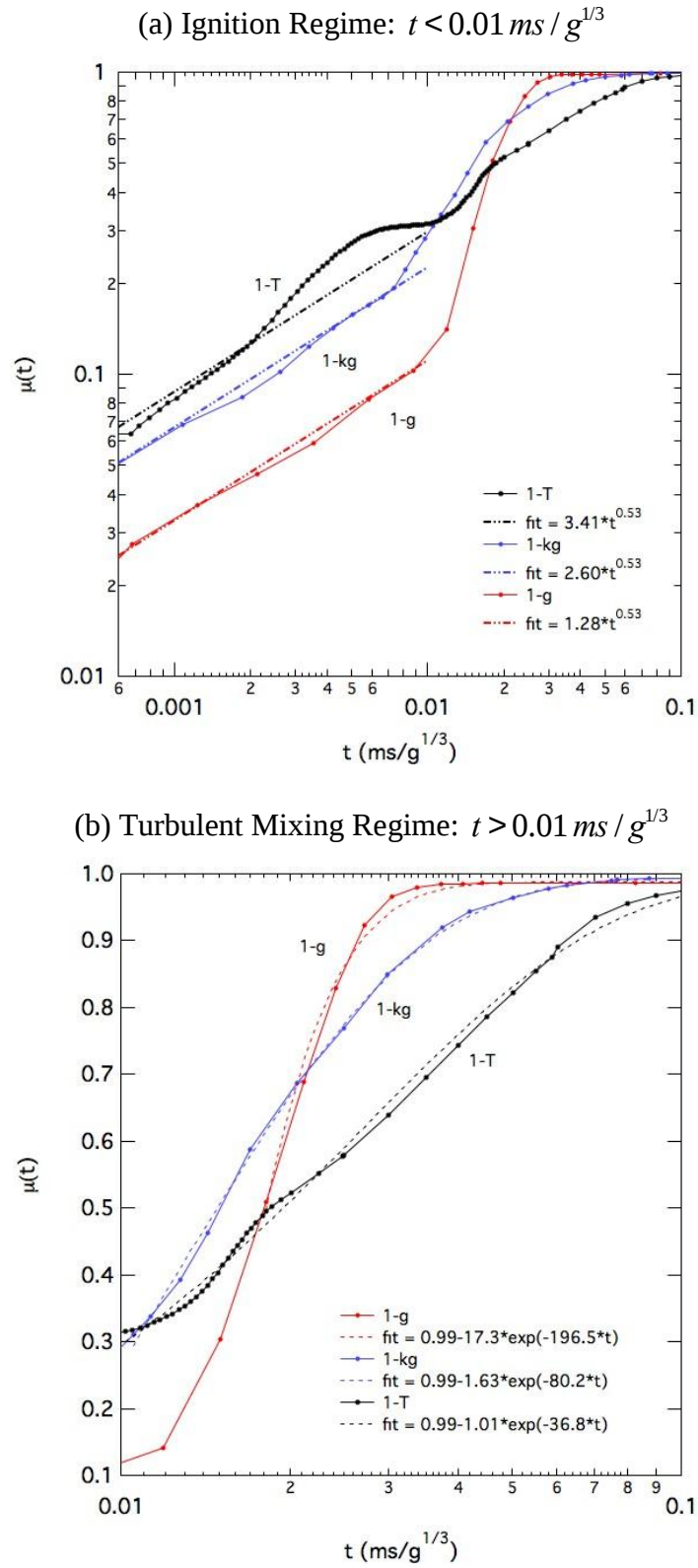


Figure 5. Fuel consumption as a function of time is depicted for various charges: (a) ignition regime: $t < 0.01 \text{ ms} / g^{1/3}$; (b) turbulent mixing regime: $t > 0.01 \text{ ms} / g^{1/3}$.