

# CLASSIFICATION OF IGNITION PROCESSES OF PREMIXED GASES

**T. Brutscher, W. Leuckel, H. Bockhorn**

Engler Bunte Institute, Combustion Technology Section,  
University of Karlsruhe (TH), Germany

## Abstract

One-dimensional ignition processes of quiescent methane-air-mixtures were investigated in detail with the simulation code INSFLA. On the basis phenomenological considerations it was possible to divide induced ignition processes in three regimes. At large radii of the external energy source the ignition process is dominated by the formation of a pool of radicals (induction time). In this regime a self-sustained flame front has been established when ignition takes place. At small radii and short times of the external energy source it is necessary to reach a critical flame ball size. At the transition between both regimes diffusion of heat and mass during the heat release of the external energy source plays an important role for the ignition process. It was possible to derive simple equations to calculate minimum ignition energies for the different regimes.

## Introduction

Currently-available simulation models of quiescent ignition processes are based on simplified conditions (one-dimensional, single-step global reaction mechanism, no radiation and heat loss to the electrodes) [1-5]. Due to these simplifications a comparison of results of ignition energies from calculations and spark discharge experiments show no satisfactory agreement [2-4]. However with parameter studies it might be possible to get more insight into the physical and chemical processes during the ignition period. Whereas experimental investigations mostly yield only global quantities (burning velocity, minimum ignition energy), the results of the simulation provide a detail picture of the spatial and temporal evolution of all species and of the temperature. This information can be helpful to develop new simplified models in which some physical and chemical effects can be neglected because of their different time scales. With these models a phenomenological description of real ignition processes such as spark discharge experiments or laser ignition experiments might be possible.

## Calculation Method

The simulation of ignition processes of methane-air-mixtures were performed using a mathematical model developed by Maas and coworkers called INSFLA. A detailed description of this model can be found in reference [1]. With this model one-dimensional, unsteady ignition and flame propagation processes under quiescent conditions can be calculated. Examples of one-dimensional geometries are an infinite cube, an infinite cylinder and a sphere. The ignition process was simulated mathematically by solving the conservation equations for total mass, species masses, momentum and energy. The conservation equations are closed by using the ideal gas law and a detailed multi species transport model of heat, mass and momentum based on the Curtis-Hirschfeld approximation. With implementation of a heat source term in the energy conservation equation the simulation of induced ignition processes is possible. The term of the artificial energy source, which has a near rectangular shape, was modelled by:

$$\dot{q} = \frac{E_Z}{V} \cdot \exp \left[ - \left( \frac{r}{r_F} \right)^8 \right] \text{ for } 0 \leq t \leq \tau_F, \quad \text{with } \dot{q} = 0 \text{ for } t > \tau_F \quad (1)$$

The user can define the energy density  $E_z/V$ , the duration and the radius of the heat source term. The calculations were performed with the uniform pressure assumption (no shock wave losses). Former mathematical investigations [1,5] show that this simplification has a neglectable effect for the investigated heating durations ( $J_F < 6$  : s). Calculations were performed using a detailed reaction mechanism consisting of 34 chemical species and 295 elementary reactions. Thermodynamic properties were taken from the JANAF tables.

## Classification of ignition processes

Numerical calculations yield a detailed picture of the spatial and temporal evolution of all species and of the temperature which allows a detailed analysis of the ignition process and of the flame front propagation. This is a strong advantage of numerical simulations in comparison to experimental approaches. In this paper we report calculations under various conditions by changing the duration, the radius and the geometry (cylinder, sphere) of the external heat source, as well as the methane concentration. When ignition takes place an excursive reduction of the oxygen concentration is observed in all simulations. The time period between the beginning of the heat release of the external energy source and the onset of the combustion process is called ignition time  $J_z$ . This time was determined for all simulations. To interpret the results, it is helpful to define non dimensional parameters with characteristic time scales. First, one can define a characteristic Fourier number  $Fo_z$  for the unsteady heat diffusion:

$$Fo_z = \frac{a \cdot \tau_z}{r_F^2}. \quad (2)$$

The non dimensional parameter describes the proportion between a characteristic diffusion time scale ( $r_F^2/a$ ) and the ignition time  $J_z$ . Another important time scale of ignition processes is the duration of the external energy source  $J_F$ . In order to get a second non dimensional parameter, it is useful to calculate the proportion of the ignition time and the duration of the energy source. In figure 1 these two parameters are plotted against each other for a set of investigated ignition processes. Three different regimes can be observed:

If the time scale at which ignition takes place is at least ten times longer than the duration of the external energy source then the Fourier number is constant and independent of the geometry, the radius and the

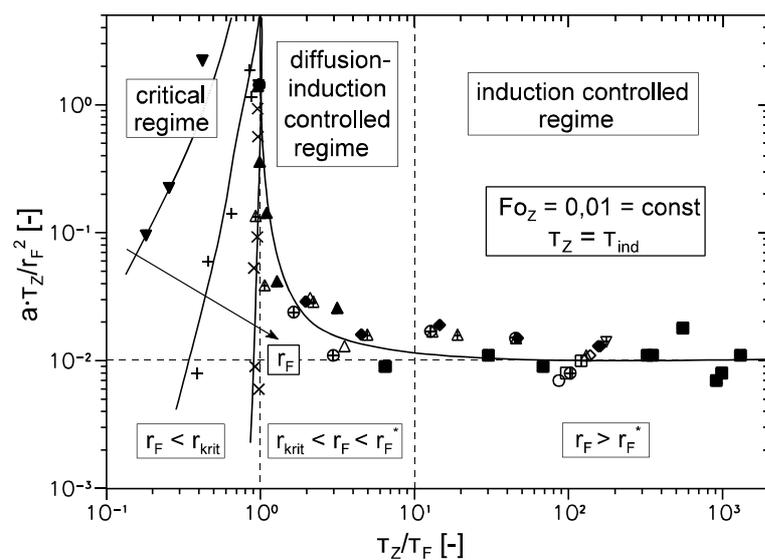


Figure 1: Classification of quiescent ignition processes with non dimensional parameters for different geometries (spherical, cylindrical), radii and durations of the external energy source as well as for different methane concentrations.

duration of the external energy source as well as of the methane concentration ( $Fo_z \cdot 0,01$ ). This regime is called **induction controlled regime**. If  $J_z/J_F$  is less than ten, the Fourier number quest for  $J_z/J_F \ll 1$  towards infinite. This regime is called **diffusion-induction controlled regime**. At very small radii and short times of the energy source the parameter  $J_z/J_F$  is smaller than one. In this so-called **critical regime** the Fourier number  $Fo_z$  varies significantly with the radius  $r_F$  and is not a suitable, characteristic, non dimensional parameter of the unsteady heat diffusion problem.

If there are large differences between the two time scales - ignition time  $J_z$

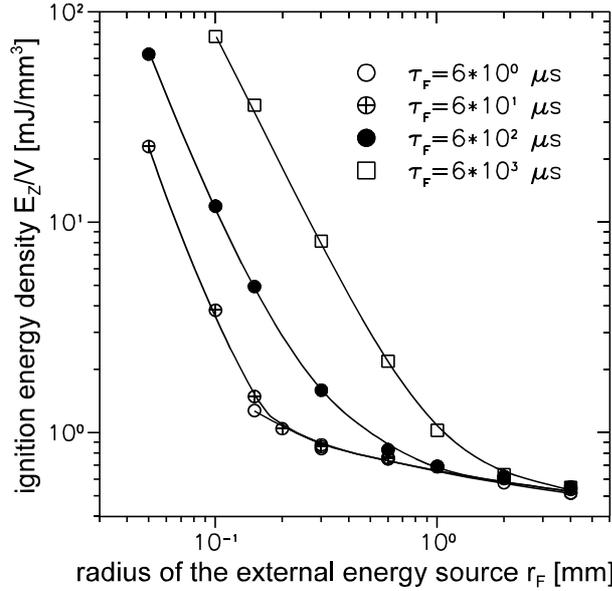


Figure 2: Ignition energy density as a function of the radius of the external energy source for different durations of the external energy source, stoichiometric mixtures, spherical geometries. equation to calculate the induction time:

$$\tau_Z \approx \tau_{ind} = A \cdot e^{\frac{B}{T_G}}. \quad (3)$$

By combining equations (2) and (3) one can derive an equation which allows to compute the gas temperature  $T_G$  to which the ignitable mixture has to be warmed up:

$$T_G \approx B \cdot \left[ \ln \left( \frac{Fo_Z \cdot r_F^2}{\alpha \cdot A} \right) \right]^{-1} \quad \text{with } Fo_Z \approx 0,01. \quad (4)$$

Thus, the ignition energy of spherical geometries in the induction controlled regime can be approximated by the equation:

$$E_{Z,Kug} = \int_{T_0}^{T_G} \frac{4}{3} \cdot \pi \cdot r_F^3 \cdot \rho_G \cdot c_{p,G} \cdot dT. \quad (5)$$

And for cylindrical geometries the ignition energy based on the length of the channel of the energy source  $l$  is given by:

$$\frac{E_{Z,Zyl}}{l} = \int_{T_0}^{T_G} \pi \cdot r_F^2 \cdot \rho_G \cdot c_{p,G} \cdot dT. \quad (6)$$

For smaller radii or shorter times of the external energy source decoupling of the two processes, ignition and heating by the external energy source, is no longer valid. Under these conditions heat conduction and diffusion during the heating period by the artificial energy source cause an expansion of the ignition kernel. In other words, during the heat release by the external energy source there are strong cooling effects by conduction and diffusion. In this regime there is a strong increase of the ignition energy densities (see figure 2). At a longer time  $J_F$  of the external energy source this increase takes place at a larger radius  $r_F$ . Criterion for minimum ignition energy is anymore a constant Fourier number, but that ignition takes place directly after the heat release by the external energy source ( $J_Z/J_F \cdot 1$ ). An estimation of the radii  $r_F^*$  at which the sharp bends in the ignition energy density curves are observed

and time of the external energy source  $J_F$  like in the induction controlled regime ( $J_Z \approx 10 J_F$ ), the two events can be decoupled. Under these conditions the duration of the external energy source has no effect on the ignition energy. A constant Fourier number in this regime demonstrates that with an increase in the radius of the external energy source  $r_F$  (extension of the unsteady cooling process) a longer ignition time  $J_Z$  and accordingly a longer induction time  $J_{ind}$  is possible to establish a self-sustained flame front. In order to get a longer induction time the gas has to be warmed up to a lower temperature  $T_G$  from the external energy source. Thus a lower ignition energy density  $E_Z/V$  is necessary. This is the explanation for the slight decrease in the ignition energy density with increased radius of the energy source. This point is clearly demonstrated in figure 2. With these observations it is possible to derive a simple mathematical model to calculate the ignition energy for the induction controlled regime. In this context we use an exponential

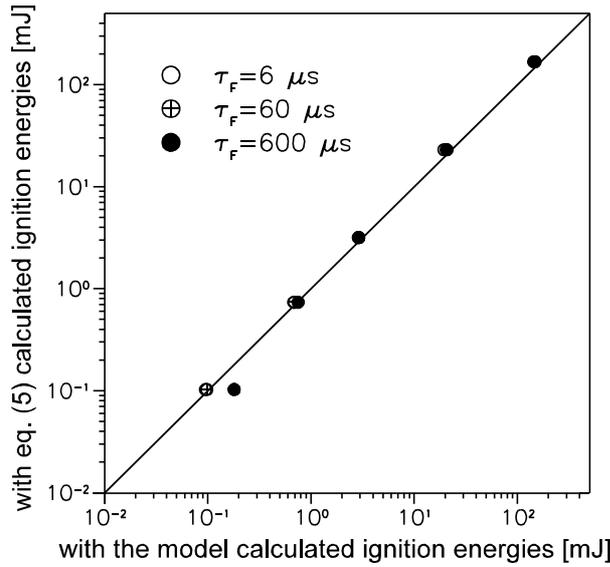


Figure 3: Comparison between ignition energies computed with equation (5) and results from the simulation code INSFLA, stoichiometric mixtures, spherical geometries.

gas kernel reaches a minimum flame ball size, which we call the critical flame front radius  $r_{krit}$ . The criterion for self sustained flame front propagation is that the time scale of the chemical heat release is equal to the time scale of a propagating flame front at this radius  $J_{kin}(r_{krit})$ . In this case the energy input from the external energy source is equal to the minimum ignition energy. A similar explanation of the ignition criterion for the critical regime can be found in [2,9]. Consequently the Fourier number for the critical regime can be formulated as follows:

$$Fo_{Z,krit} = \frac{a \cdot \tau_{kin}(r_{krit}, T_{02}, p_0)}{r_{krit}^2} \quad (8)$$

Kinetic similarity of different ignition processes requires the same value of the Fourier number  $Fo_{Z,krit}$ . This assumption can be validated by determining the radial flame front evolution using calculated concentration profiles. Thus, the critical radius as a function of the mixture strength can be deduced for spherical geometry. The critical radius was defined as the point where the turning point in the flame front evolution occurs. To determine the kinetic time scale  $J_{kin}(r_{krit})$  the tangent was deposited at the flame front curve after transgression of the critical radius. The slope of this tangent is equal to the flame front velocity. From this velocity the laminar burning velocity can be calculated as follows:

$$S_L(r_{krit}) = \frac{S_{FF}(r_{krit})}{\epsilon} \quad (9)$$

, corresponds to the expansion factor of the mixture. The kinetic time scale can be estimated as follows:

$$\tau_{kin}(r_{krit}) = \frac{a}{S_L(r_{krit})^2} \quad (10)$$

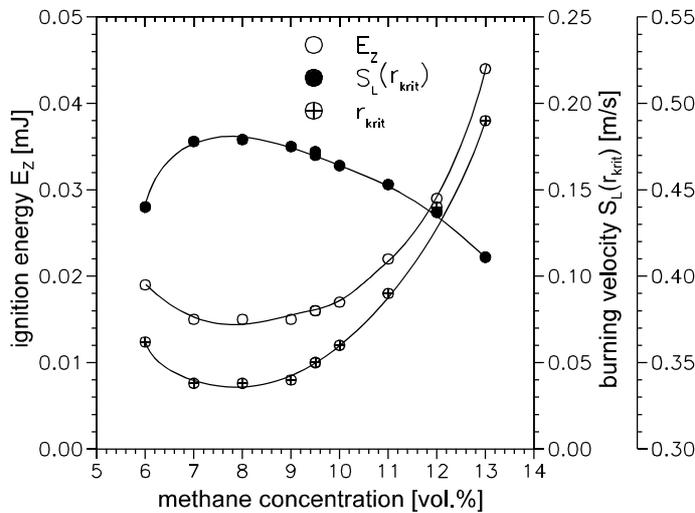


Figure 4:  $E_Z$ ,  $S_L(r_{krit})$  and  $r_{krit}$  as a function of the methane concentration.

can be made by:

$$r_F^* \approx \sqrt{1 \cdot 10^{-3} \cdot a \cdot \tau_F} \quad (7)$$

Figure 3 shows a comparison between ignition energies (spherical geometry) computed with equation (5) and results from the simulation code INSFLA. There is a good agreement between these simulations even under conditions where diffusion effects play an important role. There is also a relative good agreement between the results obtained from INSFLA simulations and from laser ignition experiments using a cylindrical heat release channel [6]. Thus, equation (5) should allow to estimate the ignition energy by laser induced ignition experiments for a cylindrical heat release channel.

It is characteristic for the critical regime that the mixture ignites before the heat release by the external energy source is terminated. A decision about successful ignition can be made if the hot

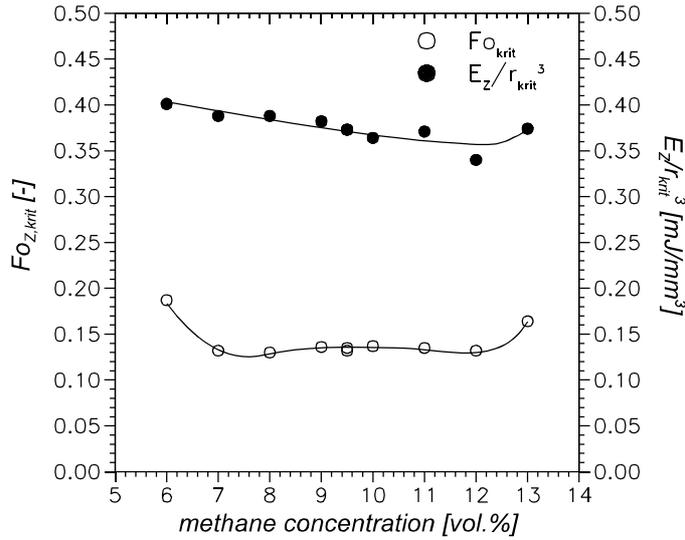


Figure 5:  $Fo_{Z,krit}$  and  $E_Z/r_{krit}^3$  as a function of the methane concentration.

$r_{krit}^3$ . So, an estimation of the ignition energy can be made by:

$$E_Z = K \cdot \rho_G \cdot c_{p,G} \cdot r_{krit}^3 \cdot \Delta T, \quad (11)$$

where  $K$  is a constant. This simple approach was used in the literature [9] to calculate minimum ignition energies from electrical spark discharge experiments. When the experimental quenching distances  $d_q$  were equated to the critical radii a good agreement was observed. Consequently, electrical spark discharge experiments could be allocated to the critical regime and equation (11) should be suited to estimate ignition energies. However, due to the additional effect of spark electrodes (heat loss, shape of the flame kernel), critical radii from spark discharge experiments are much larger than results from this work.

## References

- [1] Maas, U.; Warnatz, J.: Ignition processes in hydrogen-oxygen mixtures, *Combustion and Flame* 74: 53-69 (1988)
- [2] Sloane, T.M.: Ignition and flame propagation modeling with an improved methane oxidation mechanism, *Combust. Sci. and Tech.*, 1989, Vol. 63, pp. 287-313
- [3] Wang, C.S.; Sibulkin, M.: Comparison of minimum ignition energy for four alkanes: Effects of ignition kernel size and equivalence ratio, *Combust. Sci. and Tech.*, 1993, Vol. 91, pp. 163-178
- [4] Wu, Y.; Huang, Z.; Xiong, T.: The numerical solution of governing equations for ignition by a sphere of burned gas or spark, 20th Symposium on Combustion, 1984/pp 151-159
- [5] Frendi, A.; Sibulki, M.: Dependence of minimum ignition energy on ignition parameters, *Combust. Sci. and Tech.*, 1990, Vol. 73, pp. 395-413
- [6] Arnold, A.; Hemberger, R.; Herden, R.; Ketterle, W.; Wolfrum, J.: Laser simulation and observation of ignition processes in CH<sub>3</sub>OH/O<sub>2</sub>-mixtures, 23th Symposium on Combustion, 1990/pp 1783-1788
- [7] Arnold, J.S.; Sherburne, R.K.: Observations of the ignition and incipient flame growth in hydrocarbon-air mixtures, 4th Symposium (International) on Combustion, Williams and Wilkins, Baltimore, 1953, pp. 139-143
- [8] Ko, Y.; Arpaci, V.S.; Anderson, R.W.: Spark ignition of propane-air mixtures near the minimum ignition energy: Part I. An experimental study, *Combustion and Flame* 83: 75-87 (1991)
- [9] Lewis, B.; von Elbe, G.: *Combustion, Flames and Explosions of Gases* (Third Edition), Academic Press, New York, 1987, pp. 333ff

In figure 4 the results of  $r_{krit}$ ,  $S_L(r_{krit})$  and  $E_Z$  for different methane-air mixtures are shown. There is a minimum of  $r_{krit}$  and  $E_Z$  in the range between 7-9 % methane, and a rise to the ignition limits. In the literature one can find the same dependence of the critical radius [4,7,8] and the ignition energy [2-4,9] both from experimental and mathematical results. For  $S_L(r_{krit})$  there is a diametrical trend. Here, the maximum is at that position where the values of  $r_{krit}$  and  $E_Z$  are minimal. With these values the Fourier number  $Fo_{Z,krit}$  is almost constant (see figure 5). Consequently  $Fo_{Z,krit}$  is the characteristic non dimensional parameter of ignition processes for the critical regime. Further on, one can see that there is a correlation between the calculated ignition energy and