

DROPLETS AUTOIGNITION SIMULATIONS OF ETHANOL MIXTURES WITH A REDUCED KINETIC MECHANISM

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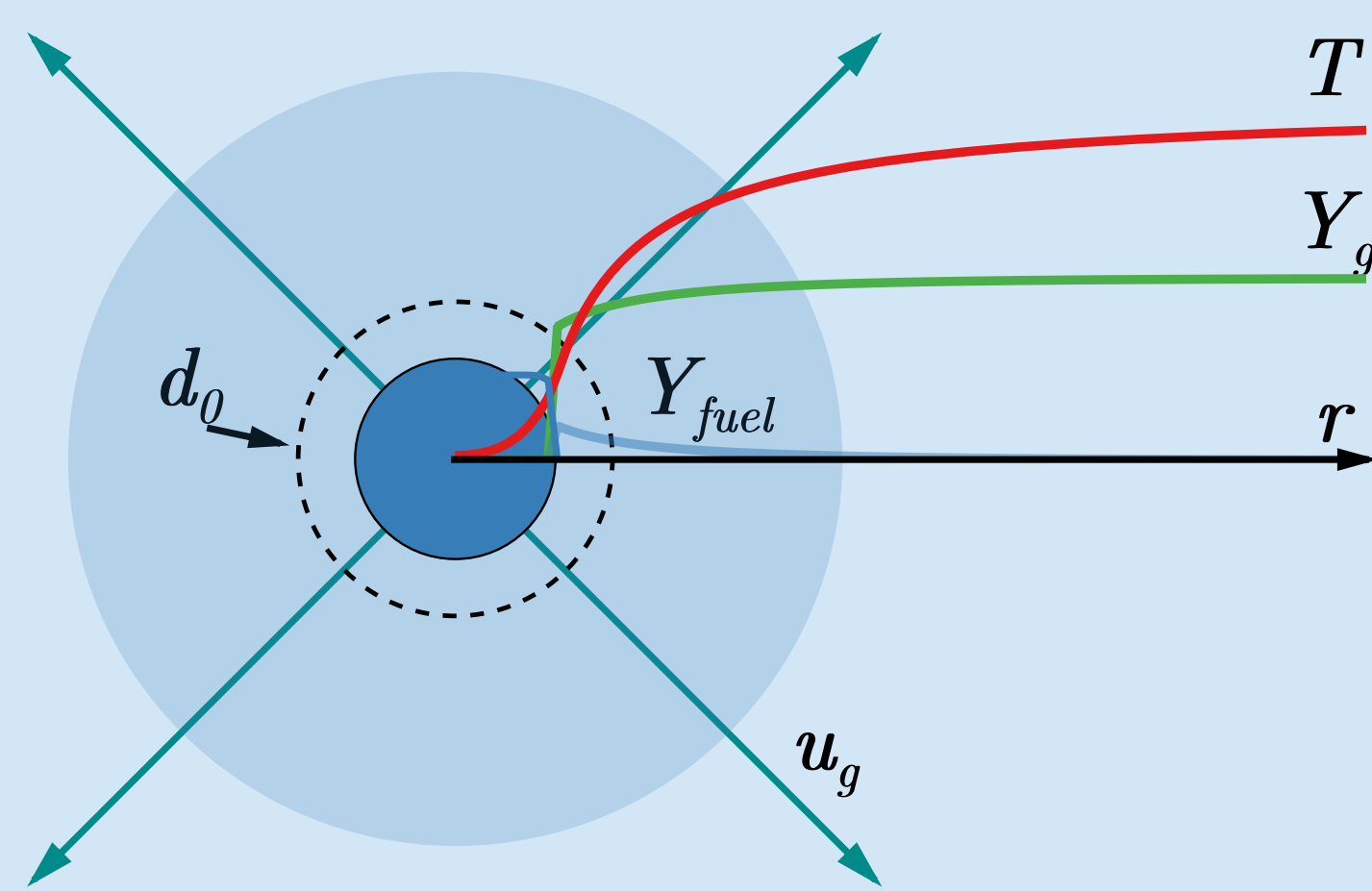
ABSTRACT

As part of a wider effort devoted to increase the basic understanding of droplet combustion, in this work we will be concerned with the analysis of the autoignition, without gravity, of an individual droplet of radius $a(t)$ in a hot air environment at a temperature $T_{g\infty}$ and a pressure p_{∞} . A mathematical 1D model has been implemented in an efficient finite-volume numerical code. The code allows the simulation of vaporization and ignition of single and multi-component fuel droplets with the implementation of a moving mesh method for droplet surface tracking.

Simple component droplets of ethanol will be numerically analyzed where special attention is given to the chemistry. A multipurpose 14-steps chemical model, previously reported, is used and compared to a 1-step Arrhenius mechanism specially developed in this work. Consideration is given to the development and test of adequate models, for molecular transport and thermodynamics in both phases, to be as accurate and computationally efficient as possible. Our computational results of a single-component droplet of ethanol show very good agreement with droplet combustion experiments.

Large quantitative differences appear when droplet autoignition times are compared with those of homogeneous gas mixtures, suggesting that, at high temperatures, autoignition is dominated by vaporization and mixing, while the chemistry is, essentially, very fast when compared to these phenomena. This is further emphasized by the reverse pressure-dependence of the autoignition times for droplets and the low equivalence ratio of the mixture when the autoignition process occurred.

FORMULATION



Conservation equations

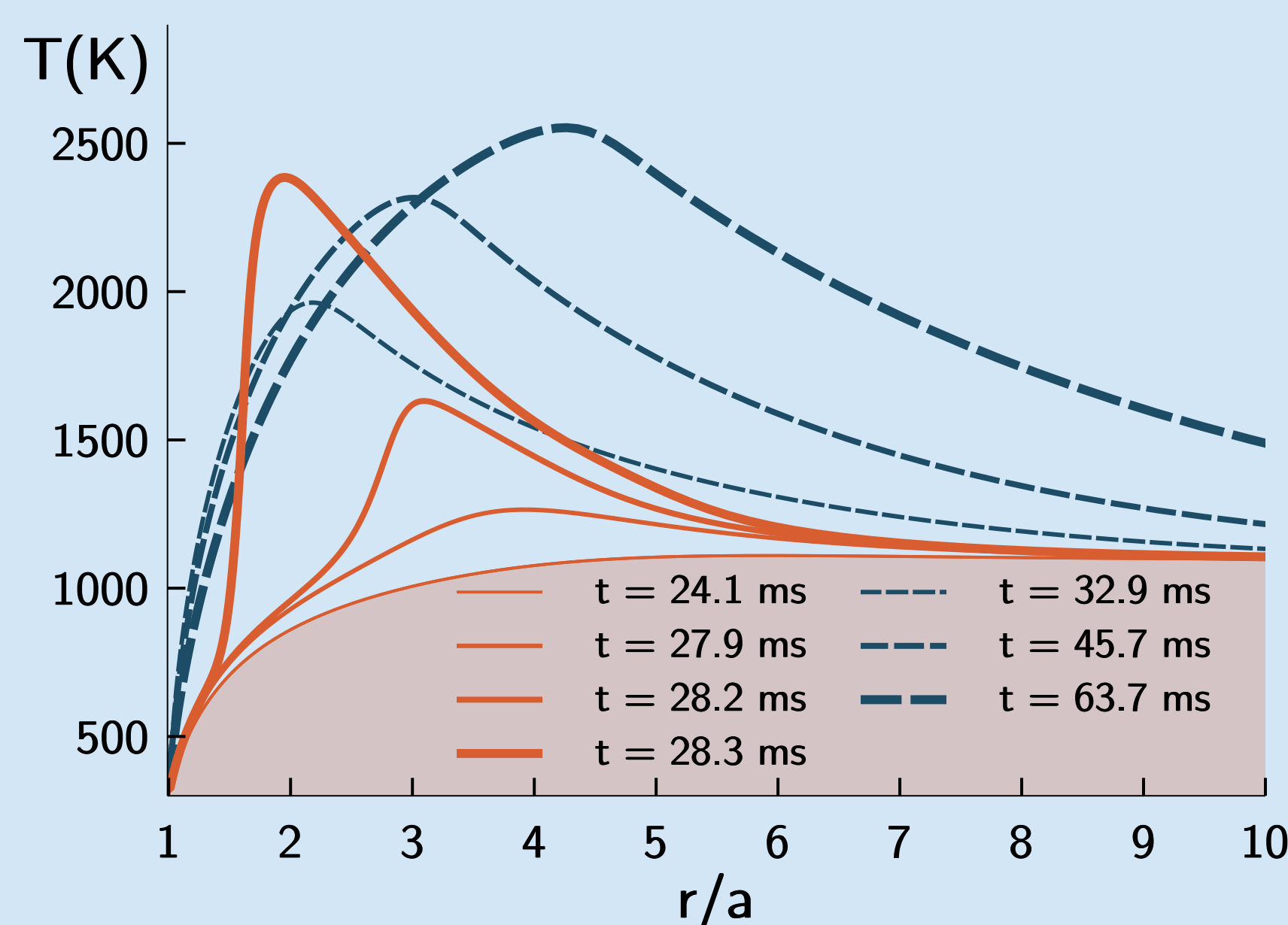
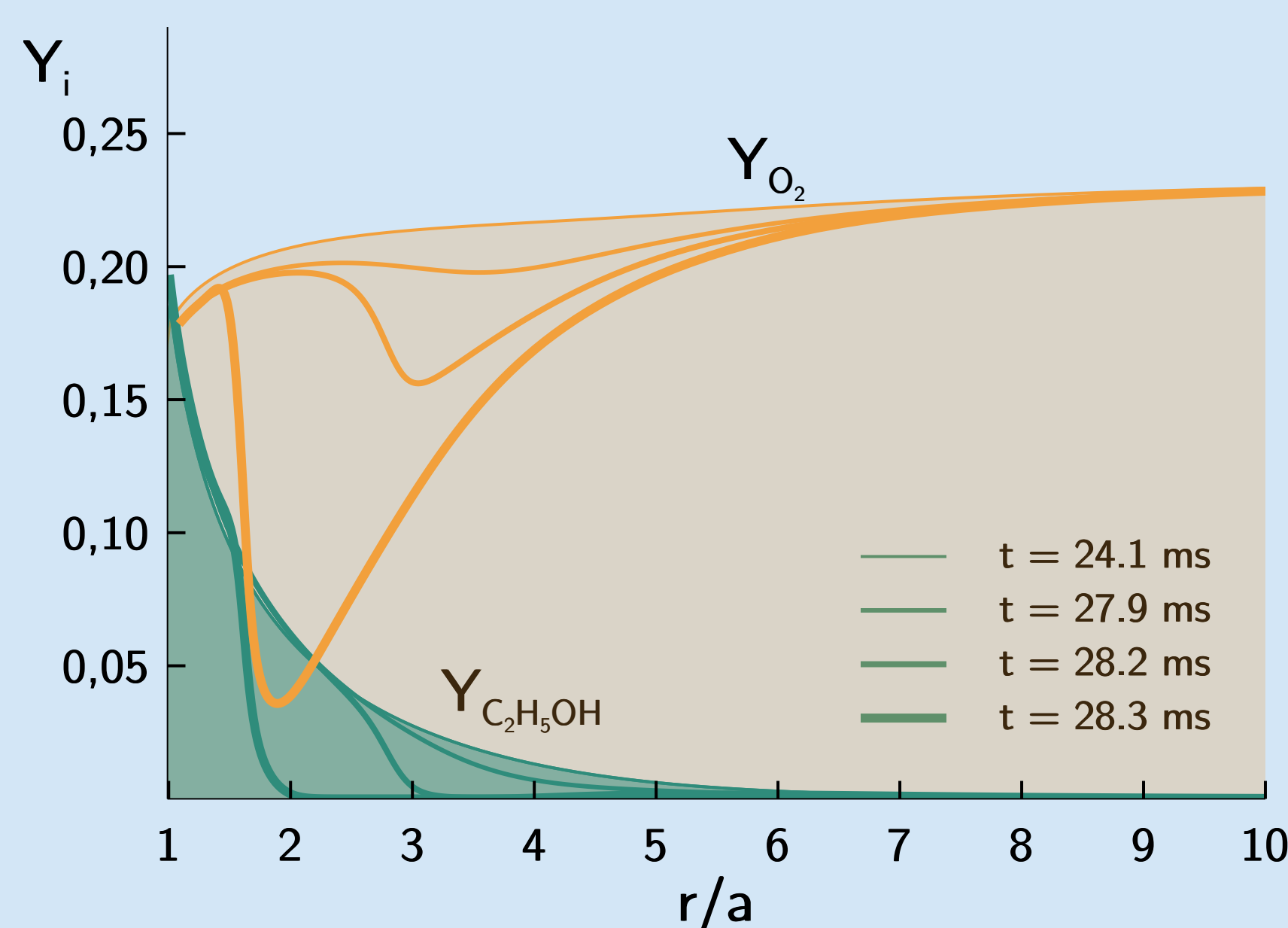
$$\begin{aligned} \frac{\partial \rho_{\beta}}{\partial t} + \nabla \cdot (\rho_{\beta} u_{\beta}) &= 0 \\ \frac{\partial (\rho_{\beta} Y_{\beta,i})}{\partial t} + \nabla \cdot (\rho_{\beta} Y_{\beta,i} u_{\beta}) &= -\nabla \cdot J_{\beta,i} + \omega_{\beta,i} \\ \frac{\partial (\rho_{\beta} h_{\beta})}{\partial t} + \nabla \cdot (\rho_{\beta} h_{\beta} u_{\beta}) &= -\nabla \cdot q_{\beta} + \omega_{\beta} \\ \forall i = 2, \dots, N_{\beta}; \quad \beta &= \begin{cases} \ell, & \text{if liquid} \\ g, & \text{if gas} \end{cases} \end{aligned}$$

Boundary conditions at the liquid-gas interface, $r = a(t)$

$$\begin{aligned} -\dot{m}''(Y_{g,i} - Y_{\ell,i})_{r=a} &= -(J_{g,i} - J_{\ell,i})_{r=a} \\ (Y_{g,i})_{r=a} &= \left(Y_{\ell,i} \frac{W_{\ell}}{W_g} \right)_{r=a} \frac{p_{\text{atm}}}{p_{\infty}} \gamma_i e^{\int_{T_{b,i}}^{T_s} \frac{L_i(T)}{RT^2} dT} \\ -\dot{m}''(Y_{g,i})_{r=a} &= -(J_{g,i})_{r=a} \\ -\dot{m}'' \sum_{i=1}^{N_l} (Y_{\ell,i} L_i(T))_{r=a} &= \left(k_g \frac{\partial T}{\partial r} - k_{\ell} \frac{\partial T}{\partial r} \right)_{r=a} \\ &\quad - \sum_{i=1}^{N_l} (J_{\ell,i} L_i(T))_{r=a} + \alpha_{\text{eff}} \sigma (T_{\infty}^4 - T_s^4) \end{aligned}$$

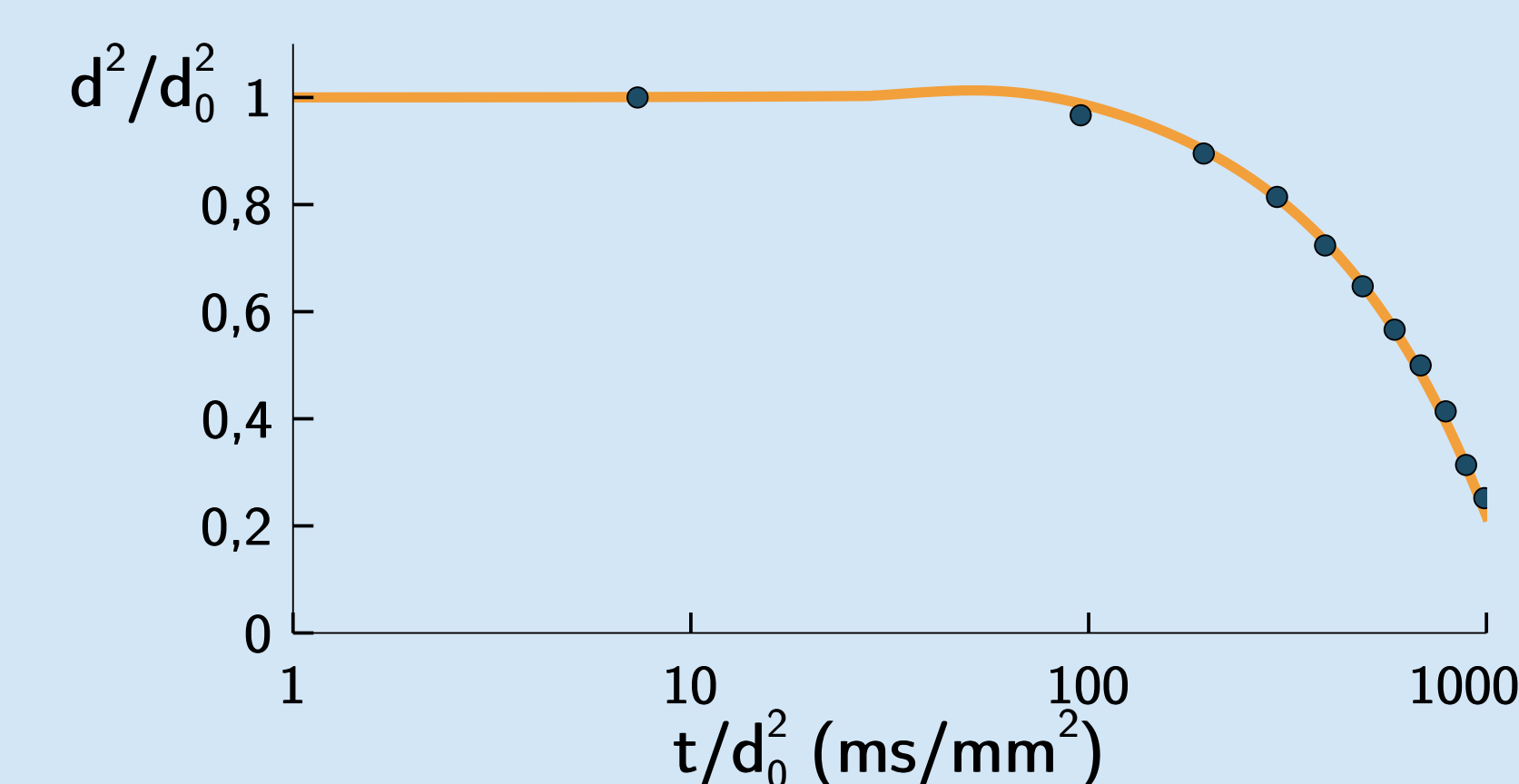
RESULTS

Temperature and mass fraction profiles

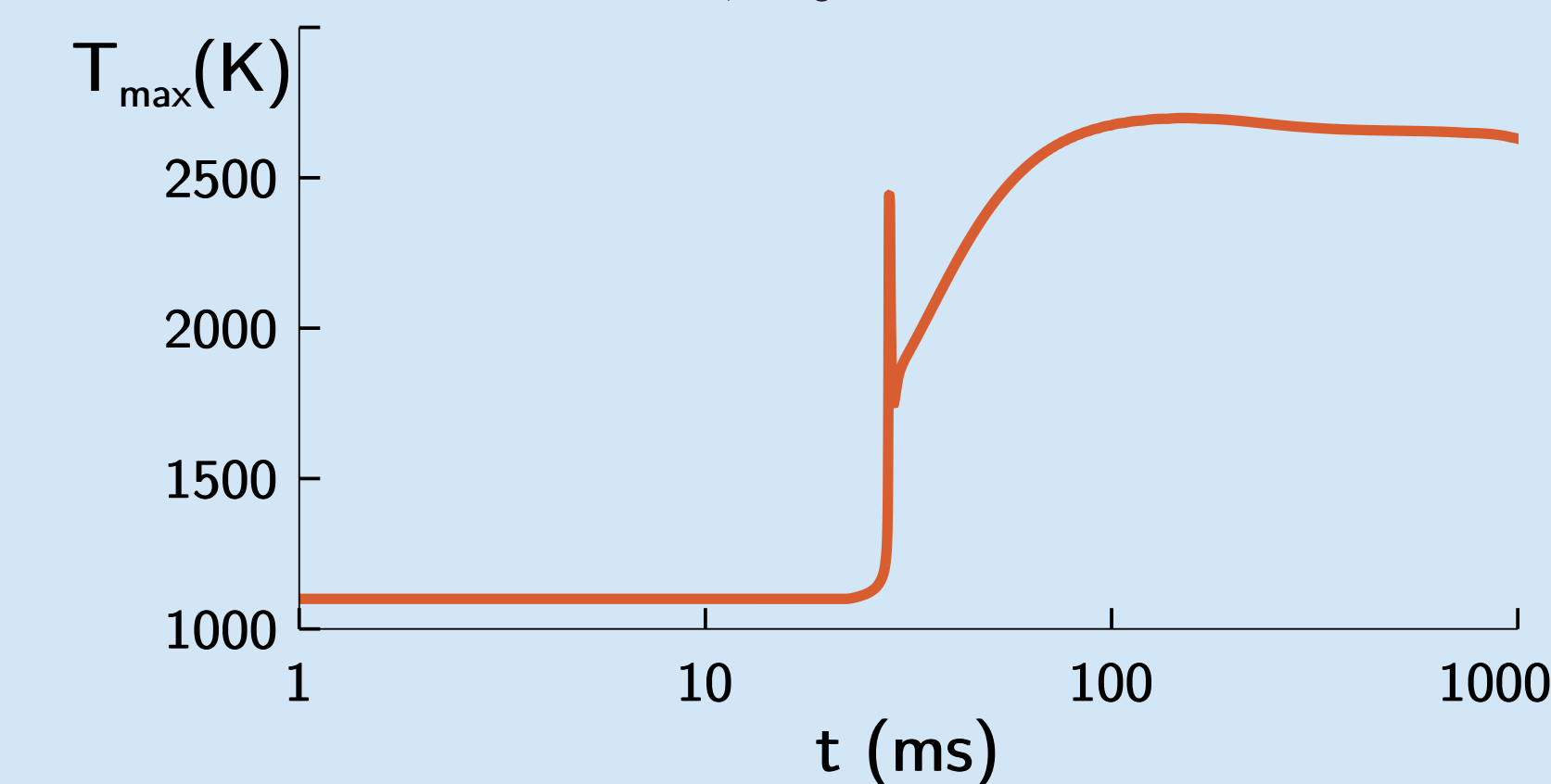


Evolution in time of temperature and mass fraction profiles as function of normalized distance r/a .

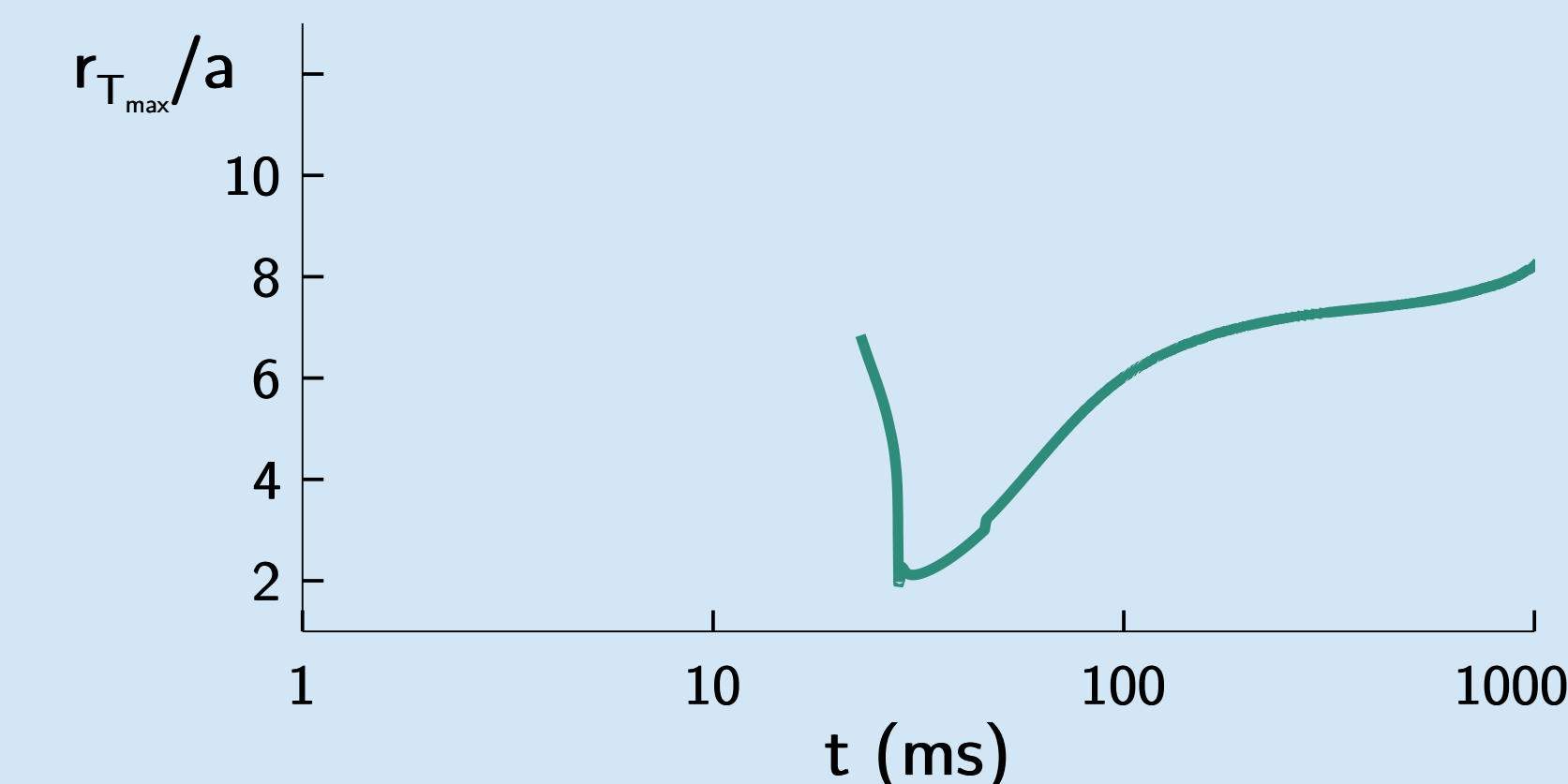
Droplet autoignition properties



Droplet normalized surface d^2/d_0^2 as function of normalized time t/d_0^2 .

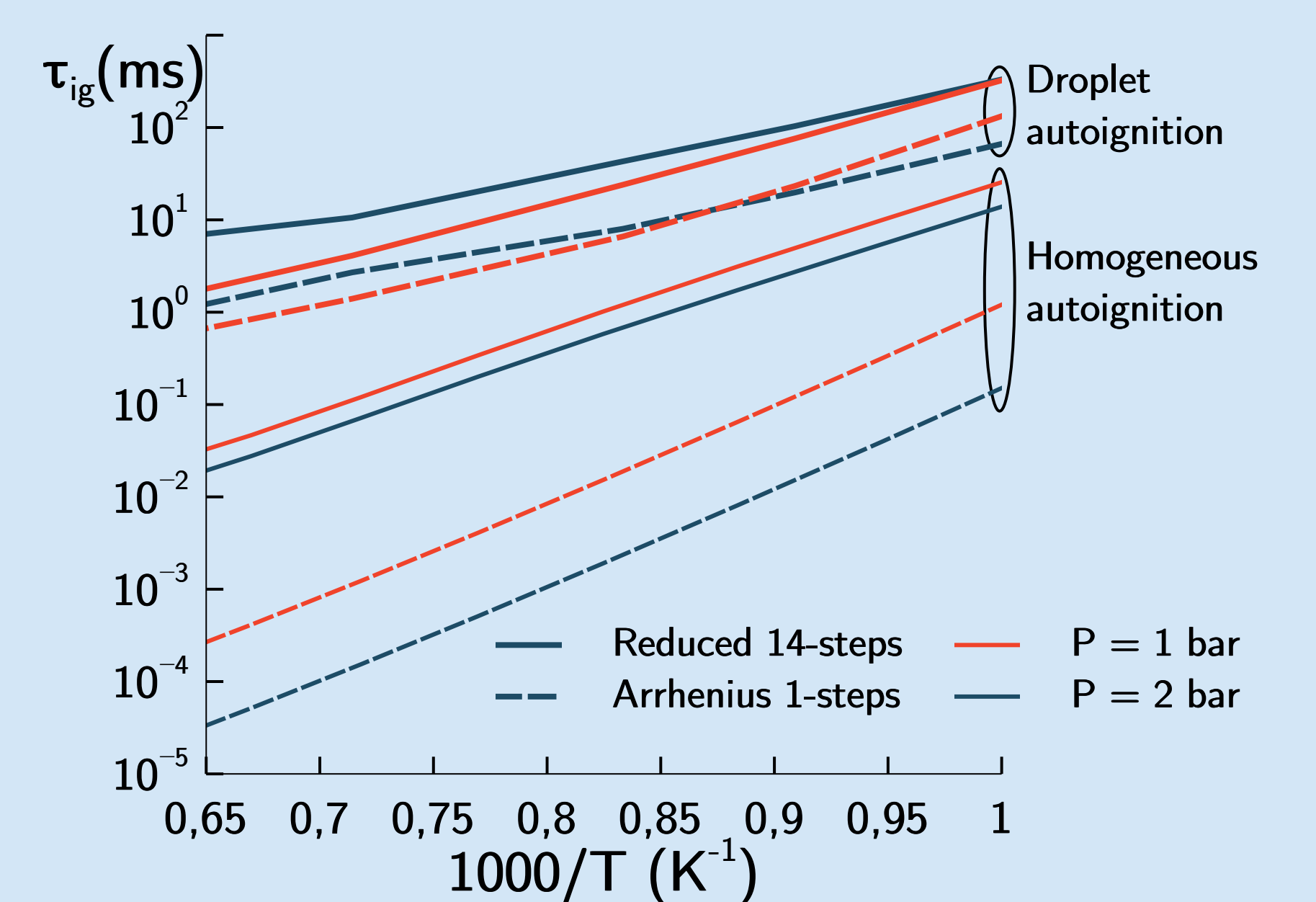


Maximum gas temperature T_{max} as function of time.

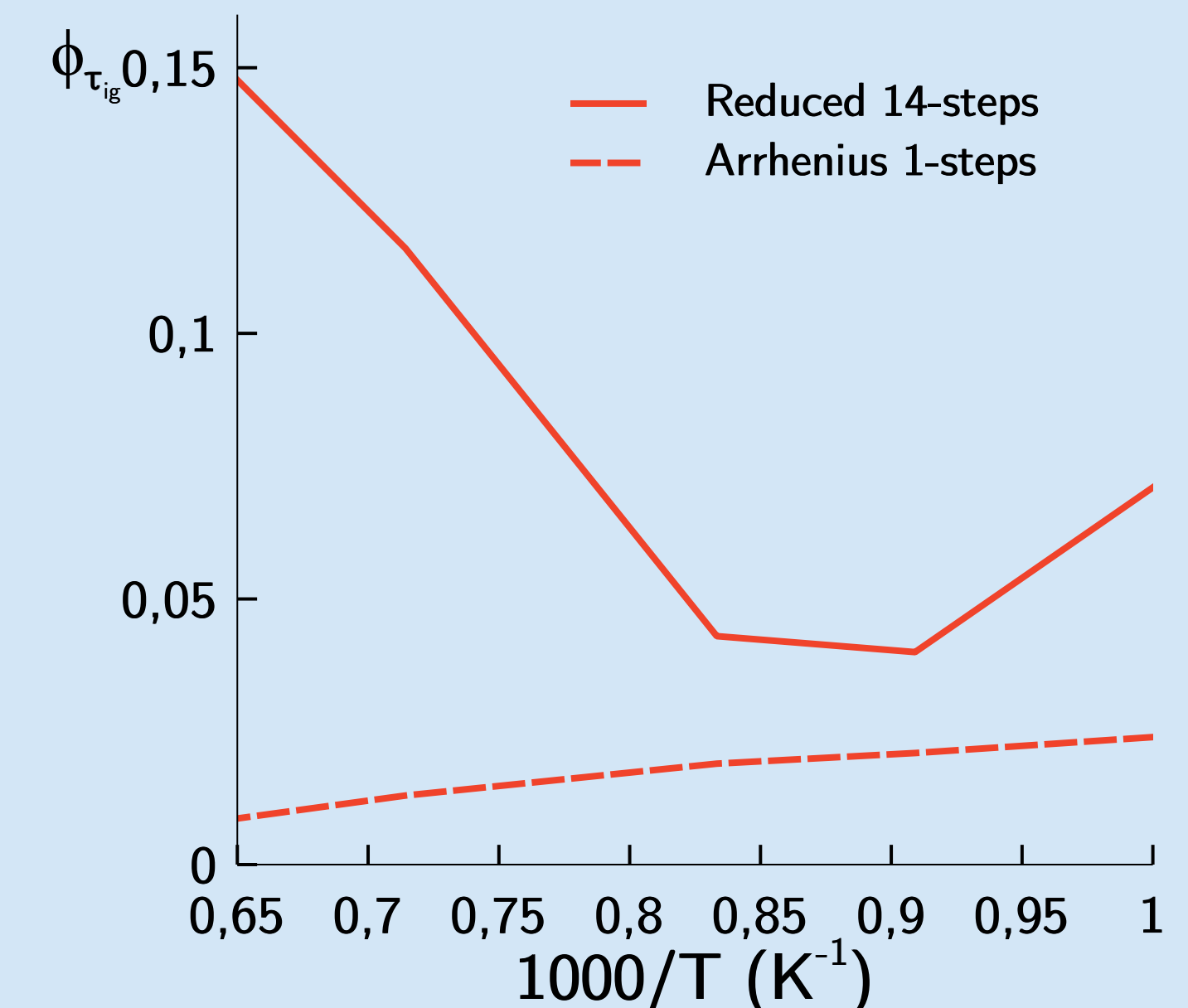


Normalized position of maximum gas temperature as function of time.

Autoignition delay times and conditions



Autoignition delay time for ethanol-air droplet and homogeneous gas mixture as function of ambient temperature T .



Equivalence ratio at the autoignition location for ethanol-air droplet as function of ambient temperature T .

Ethanol-air droplets of $d_0 = 1\text{mm}$ and $T_{d_0} = 300\text{K}$ at ambient temperature and pressure of $T_{\infty} = 1100\text{K}$ and $p = 1\text{bar}$ respectively simulated with the 1-step mechanism.

Ethanol-air droplets of $d_0 = 1\text{mm}$ and $T_{d_0} = 300\text{K}$.