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Non-steady propagation of single and counter hydrogen and methane flames in initially motionless gas

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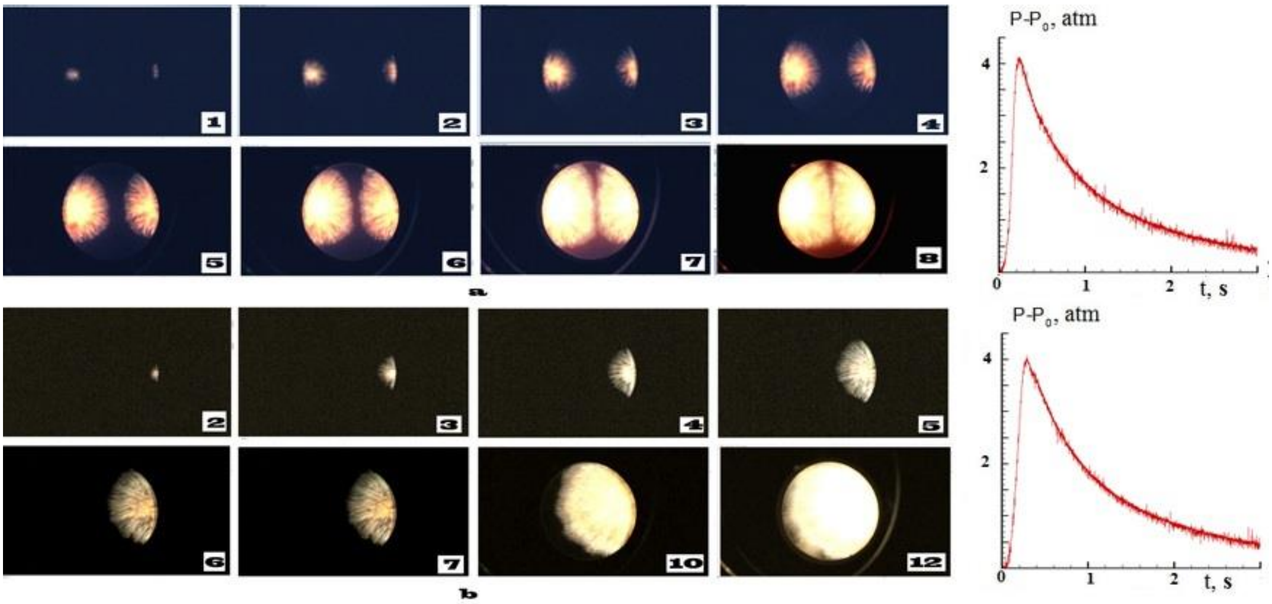

Figure S1 Speed filming of counter (a) and single (b) FF propagation in a mixture of 4% CCl_4 +12% H_2 + 84% air, P = 1 atm , 600 frames/s, at simultaneous spark initiation opposite on diameter (a) and a single spark ignition (b) at a lateral surface of reactor 4.

Calculations

$$\rho T = P \quad (1a)$$

$$\rho_t + (\rho v)_y + (\rho u)_x = 0 \quad (1b)$$

$$\rho(u_t + vv_y + uv_x) + P_y/\gamma M^2 = 1/Fr + Sc(\nabla^2 v + 1/3\, K_y) \quad (1c)$$

$$\rho(v_t + vu_y + uu_x) + P_x/\gamma M^2 = 1/Fr + Sc(\nabla^2 u + 1/3\, K_x) \quad (1d) \qquad (I)$$

$\rho\,(T_t+v\,T_y+u\,T_x) - (\gamma-1)/\gamma\,P_t - (\gamma-1)M^2\,(P_t+uP_x+vP_y) = \nabla^2 T + \beta_1 W$ (1e)

$\rho\,(C_t + v\,C_y + uC_x) = \nabla^2 C + \beta\,W$ (1f)

$W = (1-C)\exp(\zeta - \zeta/T)$ (1g)

$P_{tt} - 1/M^2\nabla^2 P = q(C_P - 1)\,\beta_1\,W_t$ (1h)

In some calculations, the reaction velocity was presented by an elementary chain mechanism: $C \rightarrow 2n$ ($w0$) and $n + C \rightarrow 2n$ + products. In this case, equations (1f), (1g) were replaced with the following ones (initial condition for concentration changes to $C_0 = 1$).

$\rho\,(C_t + v\,C_y + u\,C_x) = \nabla^2 C - \beta\,n\,W$

$\rho\,(n_t + v\,n_y + u\,n_x) = \nabla^2 n + 2\beta\,n\,W$

$W = C\exp(\zeta - \zeta/T)$

where $\nabla^2 = (...)_{yy} + (...)_{xx}$ is the two-dimensional Laplace operator, $K = v_y + u_x$ is the viscous dissipation, M is the Mach number, $P(x,y,t) = P_0(t) + \gamma M^2 p_2(x,y,t) + O(M^3)$, $P_0(t)$ is the static pressure (computed based on conservation laws [1]), $p_2(x,y,t)$ is the dynamic pressure, $P_{tt} = d^2P/dt^2$, d(...)/dt is a material derivative, u, v are the velocity components in the directions x, y, respectively, ρ is the density and T is the temperature; a chemical reaction is presented by a first-order Arrhenius reaction, C is the reagent concentration, $1 - C$ is the extent of transformation, and ζ is a dimensionless coefficient. Dimensionless parameters: Schmidt's criterion Sc = ν/D, D is diffusivity, ν is kinematic viscosity, γ is the relation of constant pressure C_P and constant volume thermal capacities; β_1 characterizes heat release allocation for concentration, β is a kinetic coefficient (proportional to Damköhler number [2]). The solution of the problem was carried out by finite element analysis by means of the package (FlexPDE 6.08, A Flexible Solution System for Partial Differential equations, 1996-2008 PDE Solutions Inc.[3]). Initiation condition was taken $T = 10$ on the boundaries of the channel. Boundary conditions were $C_x = 0$, $C_y = 0$, $n = 0$, as well as a convective heat exchange $T_t = T - T_0$, $u = 0$, $v = 0$, $\rho_x = 0$, $\rho_y = 0$.

References

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3 G. Backstrom, *Simple Fields of Physics by Finite Element Analysis*, GB Publishing, 2005.