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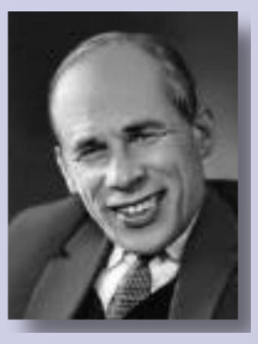

The effect of diffusion on the combustion of a sphere of polymethyl methacrylate in air.

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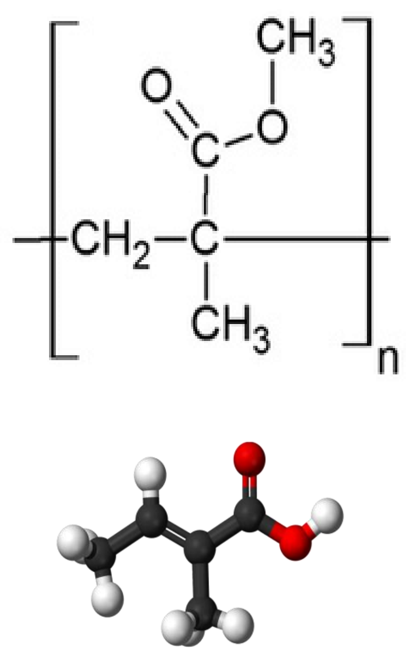
1. Introduction



Polymethyl methacrylate (PMMA) is a synthetic polymer of methyl methacrylate (MMA, $C_5H_8O_2$), a thermoplastic transparent plastic widely used in industry, construction and everyday life.

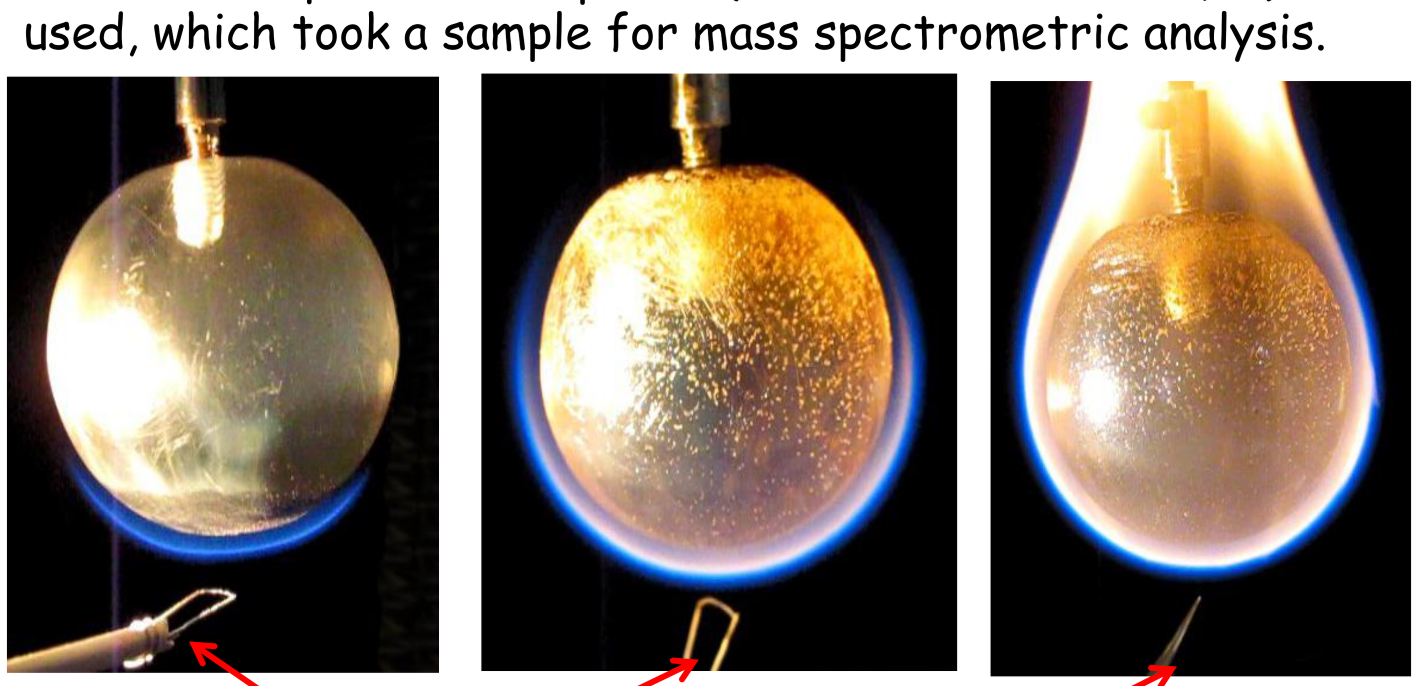
Thermal decomposition of PMMA to its methyl methacrylate (MMA) monomer occurs at temperatures above 200°C. **Methyl methacrylate** is the methyl ester of methacrylic acid.

The aim of this work is to study the influence of fuel diffusion factors on flame propagation on a curved surface under conditions of free convection.

2. Experiment

The object of research was a sphere made of cast polymethyl methacrylate (PMMA) with a diameter of 40 mm.

The sphere is placed on a movable suspension in the air under normal conditions. The ignition was carried out from below using an electric heater. To measure the thermal and chemical structure of the flame, a Pt – PtRh (10%) thermocouple 50 μm thick and a quartz microprobe (orifice diameter 60 μm) were used, which took a sample for mass spectrometric analysis.

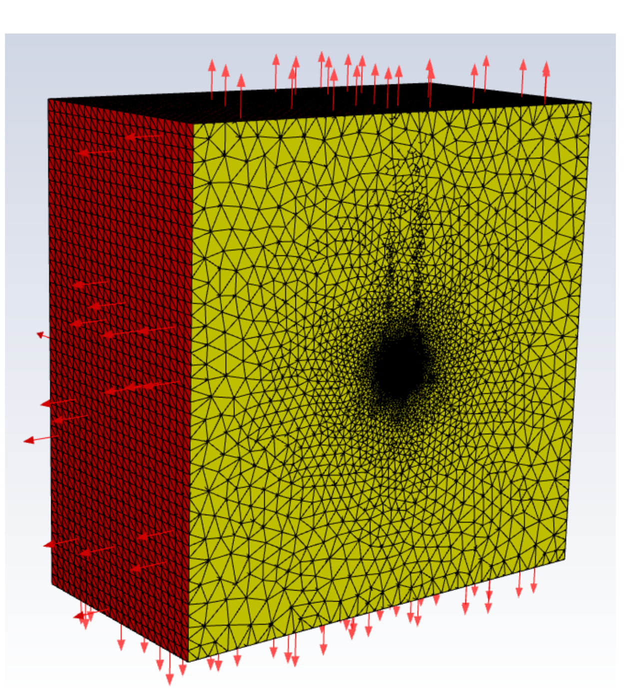


thermocouple microprobe

3. Modeling

The calculation of the gas flow around a solid body was carried out on the basis of the system of complete Navier-Stokes equations for a multicomponent mixture, supplemented by a kinetic mechanism and taking into account conjugate heat transfer and convection.(ANSYS Fluent [Academic Research, ANSYS 2021 R1, http://www.ansys.com/])

The structure of the computational grid is ≈ 5 million cells.



Computational grid

The computational domain is a square 40×40 cm, in the center of which there is a hard sphere. All boundaries of the computational domain are permeable. The air mixture is set inside the computational domain (O_2/N_2 : 0.21/0.79).

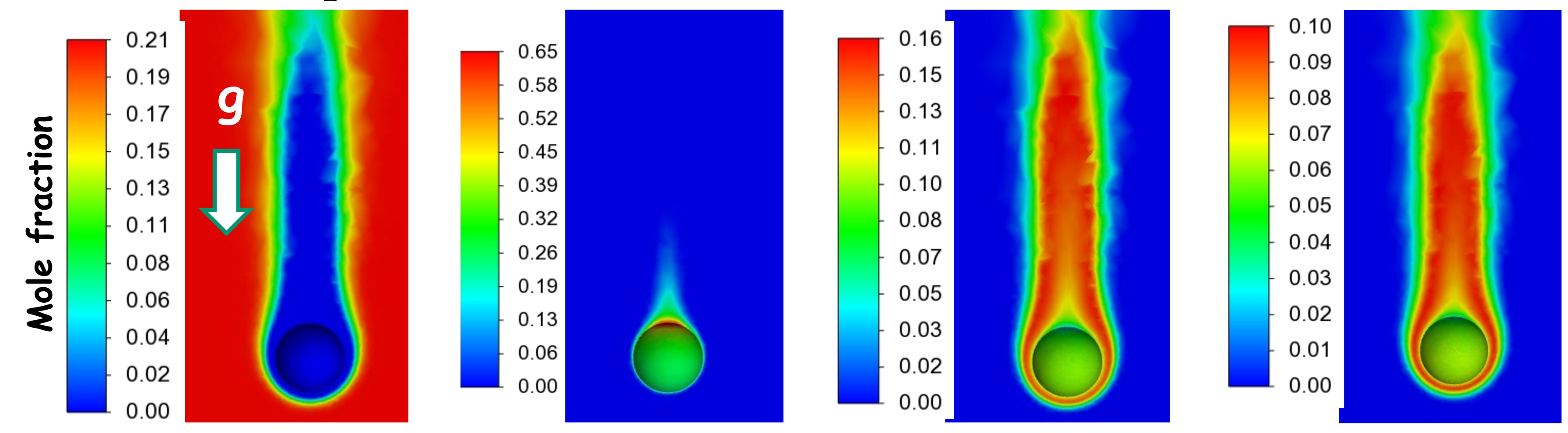
The thermophysical properties of the sphere correspond to those of PMMA. The solid-gas boundary is the conjugate boundary.

The transition of the solid phase to the gaseous phase is determined by the reaction R2 (PMMA+AC=>AC+MMA, AC- active center) of the sphere flowing on the surface. The rate of PMMA pyrolysis was described by the rate constant: $k = 6.45*10^7*e^{-29000/RT}$ [S.A. Trubachev et al., Proc.Comb.Inst. 38, 2021, 4635-4644]

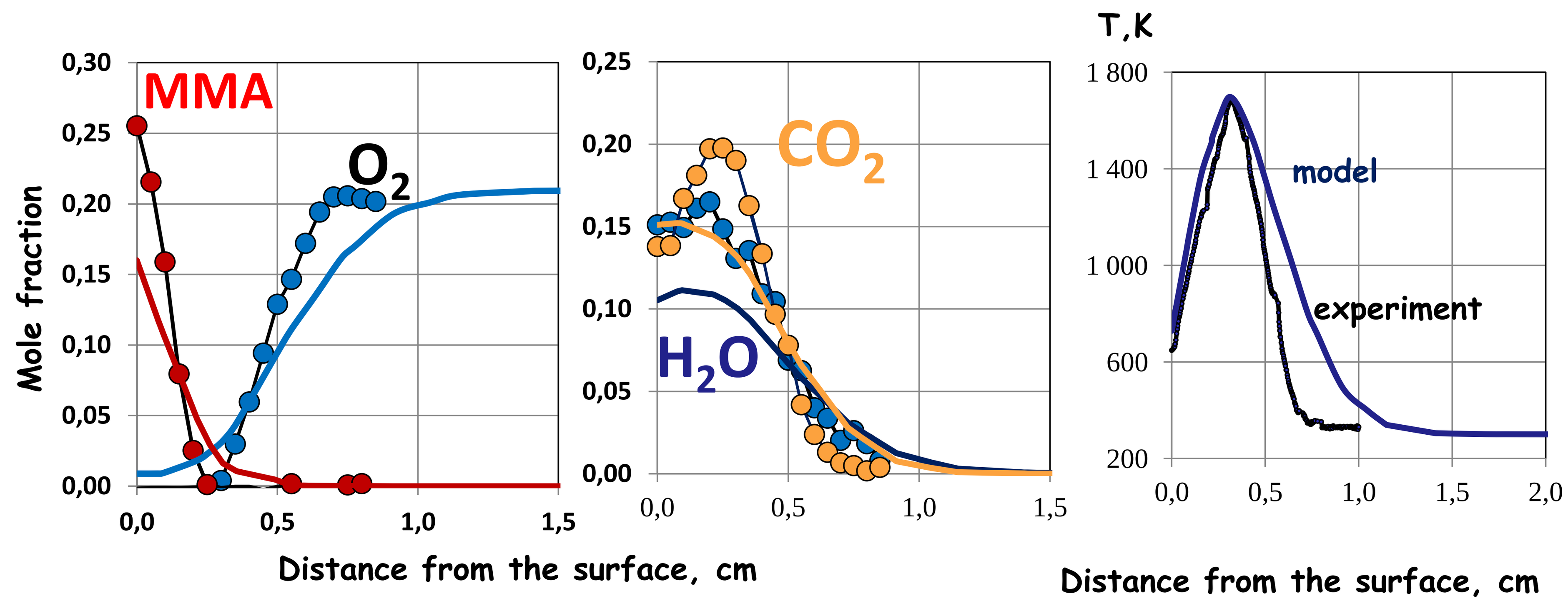
The combustion of MMA in the gas phase was described by a one-step global reaction $C_5H_8O_2 + 6O_2 \rightarrow 5CO_2 + 4H_2O$ (R1) with the rate constant $k = 1.4*10^{15}*e^{-67320/RT}$($cm^3$/(mol sec)) [K. Seshadri and F.A. Williams, J. Pol. Scien 16, 1978, 1755-1778] and with the first order reaction implied for both the fuel (MMA) and oxygen.

4. Result

Two-dimensional fields of component concentrations in a flame

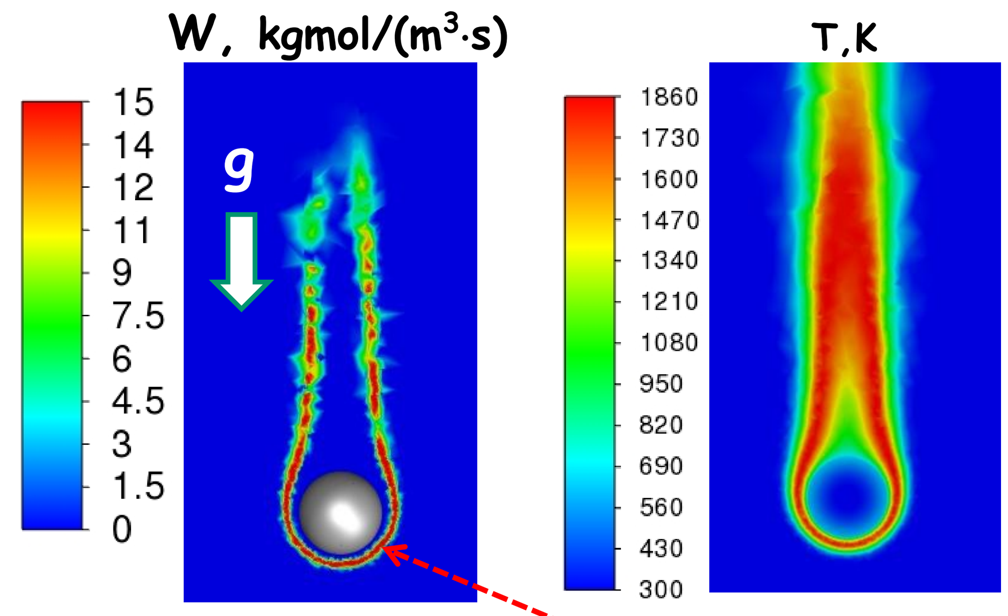


Profiles on the axis of the sphere from its surface vertically down



Symbols – experiment, lines – modeling

Reaction rate R1 and temperature field

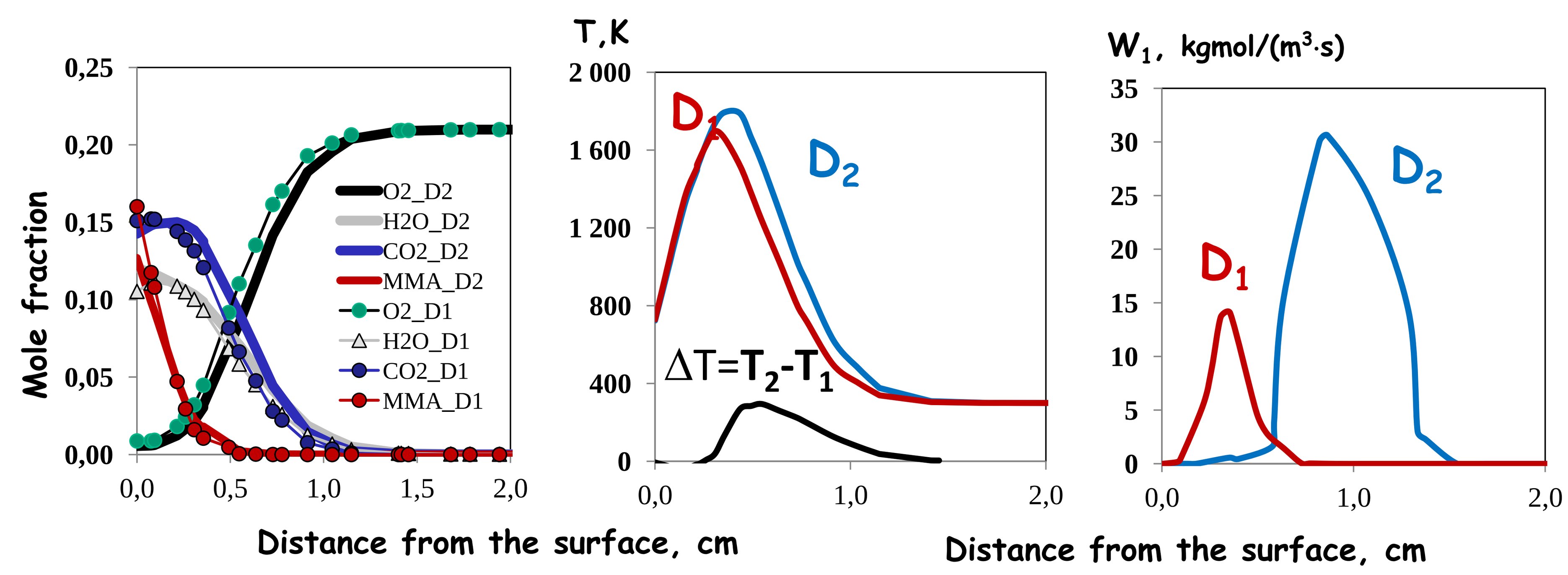


Lennard-Jones potential parameters and MMA diffusion coefficient in MMA/air mixture

N	ε/k, K	σ,Å	D_{MMA}(T=1500K), cm^2/s
1	523.2	5.664	1.32
2	280.8	3.971	2.08

$D_1 \approx 0.63*D_2$

Variation of the diffusion coefficient of MMA



$\Delta T_{max} \approx 300K$

5. Conclusion

- Comparison of the results of 3D modeling with experimental measurements showed that the proposed coupled kinetic model satisfactorily describes the thermal and chemical structure of the flame.
- Modeling showed that combustion in the gas phase takes place in a narrow spatial region.
- With an increase in the MMA diffusion coefficient, the maximum flame temperature increases, the MMA concentration near the surface decreases, and the zone of the main products and oxygen broadens.
- The change in the flame temperature with an increase in the DMMA coefficient is associated with an increase in heat release in the gas phase due to the reaction R1.
- Molecular data for calculating transfer coefficients are important parameters in CFD modeling.