Engineering combustion for gas release: emergency oxygen generators for aircraft and hydrogen generation for fuel cells

Oxygen or hydrogen, when associated with combustion, are normally used as reactants. Here, we consider combustion processes which produce these gases.

Numerical modeling of combustion stability in emergency oxygen generators[1]

Emergency oxygen for airplane passengers is typically generated by combustion of solid chemical mixtures based on sodium chlorate decomposition. Relatively low combustion temperatures and slow front propagation are characteristic features of these low-exothermic systems. Both industrial observations and prior experiments show that the combustion process is characterized by significant oscillations of the product oxygen flow rate caused by pulsating front propagation. These pulsations decrease the efficiency of oxygen generators, and their alleviation is the goal of our research.

In this work, a computer model for combustion wave propagation in gas-generating systems is developed. Reactant melting and convective heat transfer from the generated gas are key steps in the process. For this reason, we numerically investigate the effect of reactant melting on filtration combustion front propagation stability in gas generating mixtures.

The formation of melting regions is demonstrated in cases with significant convective gas-to-core heat transfer. When the latter is involved, no condensed phase temperature gradient is required to heat the core and this permits expansion of the thin melting front to a wide melting region. Numerical simulations demonstrate the oscillatory behavior of both front velocity and oxygen flow rate. It is shown that, by decreasing the effective heat of reaction, reactant melting is detrimental to combustion front stability. In accordance with prior theoretical results for simpler cases, the simulations demonstrate growth of pulsations with increasing reaction activation energy. A strong stabilization of front propagation is observed when combustion temperature reaches the melting point of reaction product. These results identify the important factors responsible for pulsating behavior of chemical oxygen generators.

Hydrogen generation via combustion enhanced by polymer gellant[2]

Hydrogen storage is considered a critical factor in the transition from fossil-fuel to hydrogen-based economy. Generation of hydrogen by combustion is of interest for fuel-cell based portable electronics and emergency power sources.

In this work, we propose novel polymer containing mixtures for hydrogen generation, which exhibit easy ignition, stable combustion, and enhanced hydrogen yield. Hydrogen generating compositions include metal fuel as an important ingredient. The polymer gellant acts as a retardant for water evaporation thus improving the contact between borohydride, metal fuel and H_2O. In equilibrium conditions, the deviations in water boiling temperature due to polyacrylamide (PAA) are insignificant (about 2°C). At heating rate 20°C/min, the gellant increases boiling temperature by ~10°C. The heating rates during hydrogen generation via combustion exceed 1000°C/min and a more significant delay in water evaporation should be expected.

The experiments with $NaBH_4/H_2O/Al/PAA$ and $NaBH_4/H_2O/Mg/PAA$ mixtures demonstrate that their combustion leads to hydrogen release and is self-sustainable when both gellant and metal fuel are present (see Figure). Gaseous hydrogen evolves during the process with yields approaching 80% from theoretically possible.

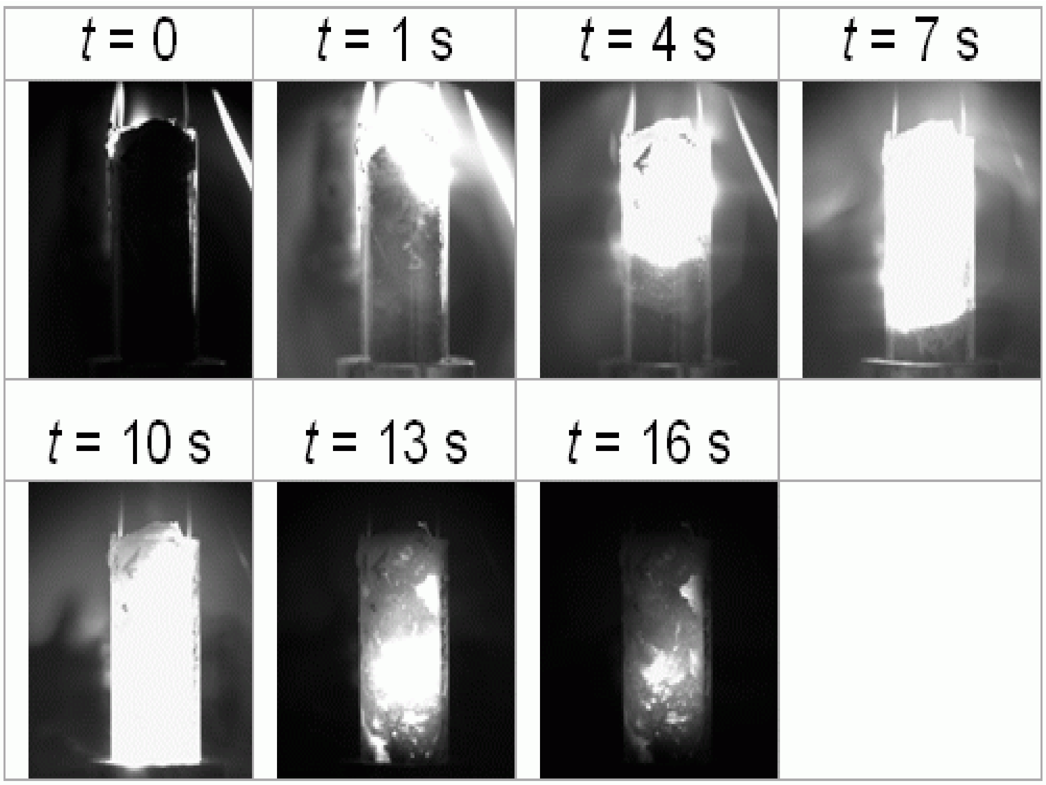

Figure: Combustion of $NaBH_4:Al:H_2O:PAA$ mixture (mass ratio 1:2:3:0.1) with hydrogen generation.

References

[1] Diakov V, Shafirovich E, Varma A. A numerical study of combustion stability in emergency oxygen generators. *AIChE Journal*. In review.

[2] Shafirovich E, Diakov V, Varma A. Combustion of novel chemical mixtures for hydrogen generation. *Combustion and Flame*. In press.