THERMOLYSIS

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Summary



Pressure (atm)	Temperature (K)	Ka	Mole fraction
			of H
0.1	1000	6.75×10^{-10}	2.09×10^{-6}
0.1	2000	3.57×10^{-3}	7.39×10^{-2}
0.1	3000	6.84×10^{-1}	6.67×10^{-1}
0.1	4000	9.53	6.67×10^{-1}
1.0	1000	$6.75 imes 10^{-10}$	1.21×10^{-6}
1.0	2000	3.57×10^{-3}	3.58×10^{-2}
1.0	3000	6.84×10^{-1}	6.46×10^{-1}
1.0	4000	9.53	6.67×10^{-1}

1. Thermolysis and Direct Thermal Decomposition

Table 1. Thermal splitting equilibrium data for water.

Table 1 gives the equilibrium constant, conversion, and mole fraction of hydrogen produced as a function of pressure and temperature. The mole fraction of water in a stoichiometric mixture of hydrogen and oxygen under thermodynamic equilibrium is shown in Figure 1 as a function of temperature and pressure. An appreciable amount of water dissociation can be obtained at very high temperatures, of the order of 2000–3000 K. At a pressure of 101.3 kPa the hydrogen mole fraction at equilibrium is 0.036 at 2000 K. By increasing the temperature to 3000 K, the hydrogen mole fraction is about 0.2 at the same pressure. Thus, the primary heat source at as high temperature as possible is preferable for one-step direct water decomposition. Such temperatures can be

reached by concentrating solar energy or by the fusion reactor. In order to produce hydrogen by direct water decomposition at lower temperature than turning temperature, work equal to ΔG is required to be supplied to the system as the separation work of hydrogen or oxygen from the gaseous products.



There are two different methods to achieve direct water decomposition preventing the recombination of active species back to water:

1. Decomposition at high temperature followed by quenching of product gases and separation of hydrogen at low temperature. In this process, the recombination of product gases, mainly hydrogen with oxygen, is prevented by a rapid quenching of the product gases from the decomposition temperature of 2000–3000 K to a temperature of 400–800 K. The quenching speed is 10^{5} – 10^{6} K s⁻¹. This can be achieved by mixing the product gases with cold water or gas.Decomposition and separation of product gases at high temperature using separation membranes. In this case, the decomposition reactor is fabricated, in part, using semi-impermeable high temperature materials. The enrichment of hydrogen or oxygen using simple membranes or the enrichment of both hydrogen and oxygen using a porous ceramic membrane is shown in Figure 2. Hydrogen is separated from the mixture of water-splitting products by gas diffusion through a porous zirconium membrane.

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Biographical Sketch

Atsushi Tsutsumi, born November 2, 1956, in Japan, is an associate professor of Chemical System Engineering at University of Tokyo. He received his Doctorate of Engineering from University of Tokyo in 1986. He has been active in research on innovative thermochemical energy technology and nonlinear dynamics and chaos scale-up methodology development for multi-phase reactors for last ten years. He has over 70 scientific publications and 100 proceedings in international journals and conferences.