Standard molar chemical exergy $\bar{e}^{CH}$ (kJ/kmol) of various substances at 298.1 K and p_0 [155]

Chemical Exergy

The chemical exergy component is associated with the work obtainable in bringing a stream of matter from the state that is in thermal and mechanical equilibrium with the environment to a state that is in the most stable configuration in equilibrium with the environment. Thus it refers to the departure of chemical composition of the system to that of the environment. The chemical state of the environment composed of a suitably selected set of environmental substances. To exclude the possibility of developing work from interactions, physical or chemical, between parts of the environment, these reference substances need to be in mutual equilibrium. Since our natural environment is not in equilibrium, it is necessary to make compromise between the physical reality and the thermodynamic theory. Based on these compromises, alternative models for calculating chemical exergies are developed [154,160,161]. In these models, the term exergy reference environment is used to distinguish the thermodynamic concept from the natural environment. For simplicity, the chemical exergy based on standard chemical exergies determined relative to a standard environment is considered in present analysis.

Standard Chemical Exergy

Standard chemical exergies are based on standard environment that consists of a set of reference substances with standard concentrations of the natural environment. As explained in the above references, the reference substances are classified in to three groups, gaseous components of the atmosphere, solid substances from lithosphere and ionic and non ionic substances from the oceans. Ahrendts [154] used restricted chemical equilibrium for nitric acid and nitrates, and unrestricted thermodynamic equilibrium for all other chemical components of the atmosphere, the oceans and a portion of the lithosphere to determine the standard chemical exergy reference environments. This model attempts to satisfy both the thermodynamic equilibrium requirements and the chemical composition of the natural environment for the gas phase. Szargut et al [161] presented a different approach where a reference substance is selected for each chemical element among the abundantly available natural environment substances that contains the elements being considered, even though the substance are not in complete stable equilibrium. The basis of this approach is that the substances found abundantly in nature have little economic value. In this approach, though the chemical composition of the exergy reference environment is closer to the composition of natural environment, the equilibrium requirement is not generally satisfied. In this work, the approach suggested by Szargut [161] is considered for analysis. Using this approach, the method to calculate standard chemical exergy and table of standard chemical exergies of substances is presented by Kotas [118].

Table G.1 gives the standard chemical exergy of some well known substances.

Table G.1 Standard Chemical Exergy of Various Substances

Substance	Formula	Model I	Model II
Nitrogen	$N_2(g)$	639	720
Oxygen	$O_2(g)$	3951	3970
Carbon dioxide	$CO_2(g)$	14176	19870
Water	$H_2O(g)$	8636	9500
Water	$H_2O(l)$	45	900
Carbon(graphite)	$C(s)$	404589	410260
Hydrogen	$H_2(g)$	235249	236100
Sulfur	$S(s)$	598158	609600
Carbon monoxide	$CO(g)$	269412	275100
Sulfur dioxide	$SO_2(g)$	301939	313400
Nitrogen monoxide	$NO(g)$	88851	88900
Nitrogen dioxide	$NO_2(g)$	55565	55600
Hydrogen peroxide	$H_2O_2(g)$	133587	-
Hydrogen sulfide	H_2S	799890	812000
Ammonia	$NH_3(g)$	336684	337900
Oxygen	$O(g)$	231968	233700
Hydrogen	$H(g)$	320822	331300
Nitrogen	$N(g)$	453821	-
Methane	$CH_4(g)$	824348	831650
Acetylene	$C_2H_2(g)$	-	1265800
Ethylene	$C_2H_4(g)$	-	1361100
Ethane	$C_2H_6(g)$	1482033	1495840
Propylene	$C_3H_6(g)$	-	2003900
Propane	$C_3H_8(g)$	-	2154000
n-Butane	$C_4H_{10}(g)$	-	2805800
n-Pentane	$C_5H_{12}(g)$	-	3463300
Benzene	$C_6H_6(g)$	-	3303600
Octane	$C_8H_{18}(l)$	-	5413100
Methanol	$CH_3OH(g)$	715069	722300
Methanol	$CH_3OH(l)$	710747	718000
Ethyl alcohol	$C_2H_5OH(g)$	1348328	1363900
Ethyl alcohol	$C_2H_5OH(l)$	1342086	1375700