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APPENDICES

Appendix A Transport Properties of Gas and Multi-component Gaseous Mixture

In the appendix A, transport properties of pure gases and multi-component gaseous mixture are summarized. The main reference that use in this appendix is from Todd and Young., 2002.

Appendix A1 Binary Diffusion Coefficient

The transport properties of gases to determine the binary diffusion coefficient that use in this model are summarized in Table A1. (Reid *et al.*, 1987 and Yakabe *et al.*, 2000)

Table A1. Value for molecular weight, σ and ε of gases

Gas	Molecular Weight (g/mol)	σ (A°)	ε
H_2	2.016	2.827	59.7
H_2O	18.015	2.641	809.1
CO	28.01	3.69	91.7
CO_2	44.01	3.941	195.2
N_2	28.014	3.798	71.4
O_2	31.999	3.467	106.7

Appendix A2 Viscosity of Pure Gas and Multi-components Gaseous Mixture

The empirical expression for determine viscosity of pure gas, μ_{gi}, is given by

$$\mu_{g_i}\left(10^{-7}\,kg/ms\right)=\sum_{k=0}^{6} b_k \tau^k , \qquad \text{(A-1)}$$

where $\tau^k = T(K)/1000$ and the values of b_k are summarized in Table A2.

Table A2. Value of b_k

Gas	b_0	b_1	b_2	b_3	b_4	b_5	b_6
H_2	15.553	299.78	-244.34	249.41	-167.51	62.966	-9.982
H_2O	-6.7541	244.93	419.50	-522.38	348.12	-126.96	19.592
CO	-4.9137	793.65	875.90	883.75	-572.14	208.42	-32.298
CO_2	-20.434	680.07	-432.49	244.22	-85.929	14.450	-0.4564
N_2	1.2719	771.45	-809.2	832.47	-555.93	206.15	-32.43
O_2	-1.6918	889.75	-892.79	905.98	-598.36	221.64	-34.754

For the viscosity of multi-component gaseous mixture, the method of Wilk is recommended and given by (Todd and Young., 2002)

$$\mu_g = \sum_{i=1}^{n} \frac{x_i \mu_{gi}}{\sum_{j=1}^{n} x_j \phi_{ij}}, \tag{A-2}$$

where μ_g is the viscosity of gaseous mixture, x_i is the molar fraction of species ith, μ_{gi} is the viscosity of species ith and ϕ_{ij} is defined as

$$\phi_{ij} = \frac{\left[1 + (\mu_i / \mu_j)^{1/2} (M_j / M_i)^{1/4}\right]^2}{8(1 + M_i / M_j)^{1/2}}, \tag{A-3}$$

Where M is the molecular weight.

Appendix A3 Thermal Conductivity of Pure Gas and Multi-component Gaseous Mixture

The empirical expression for determine the thermal conductivity of pure gas, λ_{gi}, is given by

$$\lambda_{gi}(W/mK) = 0.01\sum_{k=0}^{6} c_k \tau^k , \qquad \text{(A-4)}$$

where the values of c_k are summarized in Table A3 and τ^k is defined as

$$\tau^k = T(K)/1000 \qquad \text{(A-5)}$$

Table A3 Value of c_k

Gas	c_0	c_1	c_2	c_3	c_4	c_5	c_6
H_2	1.5040	62.892	-47.19	47.763	-31.939	11.972	-1.8954
H_2O	2.0103	-7.9139	35.922	-41.39	35.993	-18.974	4.1531
CO	-0.2815	13.999	-23.186	36.018	-30.818	13.379	-2.322
CO_2	2.8888	-27.018	129.65	-233.29	216.83	-101.12	18.698
N_2	-0.3216	14.81	-25.473	38.837	-32.133	13.493	-2.2741
O_2	-0.1857	11.118	-7.3734	6.713	-4.1797	1.491	-0.2278

For thermal conductivity of multi-component gaseous mixture, Wassiljewa's expression is recommended and given as

$$\lambda_g = \sum_{i=1}^{n} \frac{x_i \lambda_{gi}}{\sum_{j=1}^{n} \lambda_{gj} A_{ij}} , \qquad \text{(A-6)}$$

where λ_g is the thermal conductivity of multi-component gaseous mixture, x_i is the molar fraction of species ith and A_{ij} is defined as

$$A_{ij} = \frac{\left[1 + (A_i / A_j)^{1/2} (M_j / M_i)^{1/4}\right]^2}{8(1 + M_i / M_j)^{1/2}} , \qquad \text{(A-7)}$$

where M is the gas molecular weight.

Appendix A4 Isobaric Heat Capacity

The empirical expression for determine the isobaric heat capacity of pure gas, C_{pi}, is given by

$$C_{pi}(kJ/Kmol\cdot K)=\sum_{k=0}^{6}a_k\tau^k\ , \qquad \text{(A-8)}$$

where the value of a_k are summarized and τ^k is defined as

$$\tau^k = T(K)/1000 \qquad \text{(A-9)}$$

Table A4 Value of a_k

Gas	a_0	a_1	a_2	a_3	a_4	a_5	a_6
H_2	21.157	56.036	-150.55	199.29	-136.15	46.903	-6.4725
H_2O	37.373	-41.205	146.01	-217.08	181.54	-79.409	14.015
CO	30.429	-8.1781	5.2062	41.974	-66.346	37.756	-7.6538
CO_2	4.3669	204.6	-471.33	657.88	-519.9	214.58	-35.992
N_2	29.027	4.8987	-38.040	105.17	-113.56	55.554	-10.35
O_2	34.85	-57.975	203.68	-300.37	231.72	-91.821	14.776

For the multi-component gaseous mixture, the isobaric heat capacity is determined as follow

$$C_p(T)=\sum_{i=1}^{n}x_iC_{pi}(T), \qquad \text{(A-10)}$$

where x_i and C_{pi} are the molar fraction and of heat capacity of ith component.

Appendix B Thermodynamic of SOFC Reactions

In this appendix, the thermodynamic of reactions that considered in this work are presented and summarized.

Appendix B1 Enthalpy of Reactions

The empirical expression for determine enthalpies of electrochemical and chemical reactions that are considered in this work is given as

$$\Delta H_{rxn,T}\left(KJ \cdot Kmol^{-1}\right)=\sum_{k=0}^{5} a_k \tau^k , \qquad \text{(B-1)}$$

where τ^k is defined as

$$\tau^k = T(K)/1000 , \qquad \text{(B-2)}$$

where a_k is the constant depending on the reactions and are summarized in Table B1.

Table B1 Value of a_k

Reaction	a_0	a_1	a_2	a_3	a_4	a_5
H_2 oxidation	-239113	-7.53	-8.6x10^{-3}	13.33x10^{-6}	-7x10^{-9}	13.5x10^{-13}
CO oxidation	-278797	-24.1	42.77x10-3	-34.69x10^{-6}	14.8x10^{-9}	-25.6x10^{-13}
Water-gas shift	-259849	-16.554	51.3x10^{-3}	-47.9x10^{-6}	21.8x10^{-9}	-39.1x10^{-13}

Appendix B2 Standard Gibb's Free Energy of Reactions

The empirical expression for determine Gibb's free energy of electrochemical reactions of H_2 and CO is given as

$$\Delta G^0{}_{rxn,T}\left(KJ \cdot Kmol^{-1}\right)= b_0 + b_1 \ln T + b_2 T + b_3 T^2 + b_4 T^3 + b_5 T^4 + b_6 T^5 , \qquad \text{(B-3)}$$

where b_0, b_1,..., b_6 are summarizes in Table B2.

Table B2 Value of b_0, b_1,..., b_6

Reaction	b_0	b_1	b_2	b_3	b_4	b_5	b_6
H_2 oxidation	-239133	7.53	-10.79	$8.567\text{x}10^{-3}$	$-6.64\text{x}10^{-6}$	$2.34\text{x}10^{-9}$	$-3.4\text{x}10^{-13}$
CO oxidation	-282394	24.08	-50	$-42.8\text{x}10^{-3}$	$17.3\text{x}10^{-6}$	$-4.93\text{x}10^{-9}$	$6.4\text{x}10^{-13}$

For the Gibb's free energy of water-gas shift reaction, the semi-empirical expression is given as

$$\Delta G^0_{wgs,T} = \sum_{k=1}^{5} c_k T^k \, , \tag{B-4}$$

where constant c_k are summarized in Table B3.

Table B3 Value of c_k

Reaction	c_1	c_2	c_3	c_4	c_5
Water-gas shift	252	-0.794	$0.887\text{x}10^{-3}$	$-0.492\text{x}10^{-6}$	$0.104\text{x}10^{-9}$

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