Thermodynamic and transport properties of fluids and solids in a Cu-Cl solar hydrogen cycle

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ABSTRACT

Sustainable methods of clean fuel production are needed in the face of depleting oil reserves and the need to reduce carbon dioxide emissions. The technology of fuel cells for electricity production or the transport sector is already developed. However, a key missing element is a large-scale economical method of hydrogen production. The Cu-Cl thermochemical cycle is a promising thermochemical cycle to produce hydrogen. This paper focuses on a copper-chlorine (Cu-Cl) cycle and solar hydrogen production technology and describes the models how to calculate thermodynamic and transport properties. This paper discusses the mathematical model for computing the thermodynamic properties for pure substances and their mixtures such as CuCl in the solid phase with an aid of statistical thermodynamics and kinetic theory. The developed mathematical model takes into account vibrations of atoms in molecules and intermolecular forces. This mathematical model can be used for the calculation of thermodynamic properties of polyatomic crystals on the basis of the Einstein and Debye equations. We developed the model in the low temperature and high temperature region. All analytical data are compared with experimental results and these show good agreement. For the transport properties we have used kinetic theory. For fluid phase we have calculated viscosity and thermal conductivity on the basis of the Chung-Lee-Starling kinetic model, for the solid phase we have developed a model for calculations of thermal conductivity on the basis of electron and phonon contributions.

1. THERMOCHEMICAL HYDROGEN PRODUCTION CYCLE

Rather than deriving hydrogen from fossil fuels, a promising alternative is the thermochemical decomposition of water. Electrolysis is a proven, commercial technology that separates water into hydrogen and oxygen using electricity. Net electrolysis efficiencies (including both electricity and hydrogen generation) are typically about 24%. In contrast, thermochemical cycles to produce hydrogen promise heat-to-hydrogen efficiencies up to approximately 50%. This article examines the thermophysical properties of a specific cycle called the copper-chlorine (Cu-Cl) cycle, with particular relevance to nuclear-produced hydrogen. Some important components attended in Cu-Cl cycle are shown in Table 1 and Table 2. A conceptual schematic of the Cu-Cl cycle is shown in Fig. 1.

In the Cu-Cl cycle, water is decomposed into hydrogen and oxygen through intermediate Cu-Cl compounds [1, 2]. Nuclear-based "water splitting" requires an intermediate heat exchanger between the nuclear reactor and hydrogen plant, which transfers heat from the reactor coolant to the thermochemical cycle. An intermediate loop prevents exposure to radiation from the reactor coolant in the hydrogen plant, as well as corrosive fluids in the thermochemical cycle entering the nuclear plant.

Table 1: Fundamental thermophysical properties for selected Cu-Cl components:

	HCl	CuCl	$CuCl_2$	Cu_2OCl_2	CuO
	Hydrochloric acid	Cuprous chloride	Cupric chloride	Copper oxychloride	Cupric oxide
Molecular weight /kg/kmol	36.4606	98.999	134.451	214	79.545

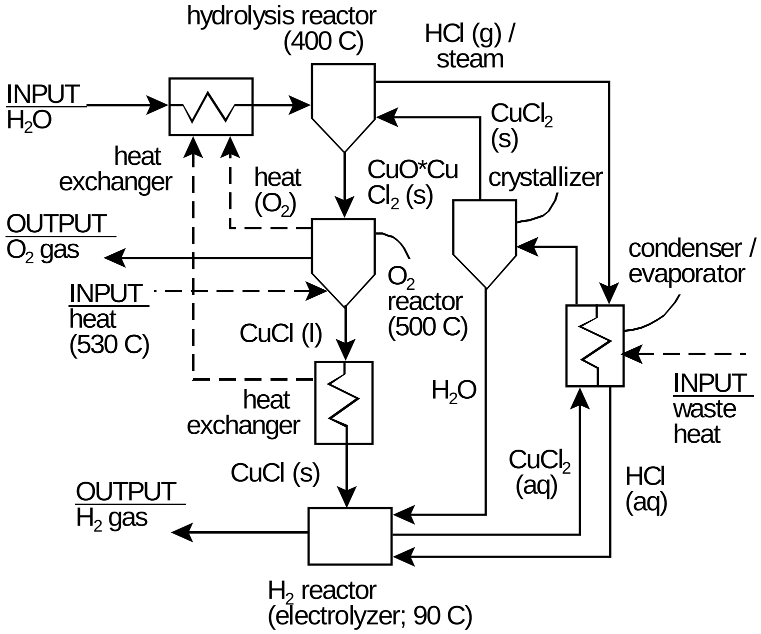

Fig. 1: Schematic of the copper-chlorine cycle for thermochemical hydrogen production [1]

Table 2: Chemical reactions in the Cu-Cl cycle [1]

Step	Reaction	Temp. Range /°C	Feed/Output (note: Q – thermal energy, V – electrical energy)	
1	$2Cu(s) + 2HCl(g) \rightarrow$ $CuCl(l) + H_2(g)$	430-475	Feed: Output:	Electrolytic Cu + dry HCl + Q H_2 + CuCl(l) salt
2	$2CuCl(s) \rightarrow 2CuCl\ (aq)$ $\rightarrow CuCl_2(aq) + Cu(s)$	Ambient (electrolysis)	Feed: Output:	Powder/granular CuCl and HCl + V Electrolytic Cu and slurry containing HCl and $CuCl_2$
3	$CuCl_2(aq) \rightarrow CuCl_2(s)$	< 100	Feed: Output:	Slurry containing HCl and $CuCl_2$ + Q Granular $CuCl_2$ + H_2O/HCl vapours
4	$2CuCl_2(s) + H_2O(g) \rightarrow$ $CuO \times CuCl_2(s) + 2HCl(g)$	400	Feed: Output:	Powder/granular $CuCl_2$ + $H_2O(g)$ + Q Powder/granular $CuO \times CuCl_2$ + 2HCl (g) Q ~ 117 kJ/mol H_2
5	$CuO \times CuCl_2(s) \rightarrow$ $2CuCl(l) + 1/2O_2(g)$	500	Feed: Output:	Powder/granular $CuO \times CuCl_2(s)$ + Q Molten CuCl salt + oxygen Q ~ 130 kJ/mol H_2

2. SOLAR HYDROGEN PRODUCTION

A significant advantage of using nuclear thermal energy to satisfy the heat requirement of thermochemical water splitting cycles is the higher energy intensity of nuclear energy per unit land area than that of solar energy. However, most currently existing thermochemical hydrogen production cycles require a temperature of higher than 500^{o}C [3-10], which cannot be satisfied by current large scale nuclear reactors, although potentially can be satisfied by future generation nuclear reactors (i.e., Gen-IV reactors) [11, 12]. Table 3 lists some typical hybrid fully thermal and thermal chemical hydrogen production cycles other than the aforementioned Cu-Cl cycle. It can be observed that the temperature requirements of some cycles are even higher than that can be provided by Gen-IV reactors. Therefore, using high temperature solar thermal energy that is obtained from concentrated solar irradiance has become another promising option.

Table 3. Temperature requirements of some thermochemical hydrogen production cycles

No.	**Cycle** [reference]	**Thermal / Electrolytic**	**T/ ºC**	**Chemical reactions**
1	Ispra Mark 13 [5]	Thermal	850	$2H_2SO_4(g) = 2SO_2(g) + 2H_2O(g) + O_2(g)$
		Electrolytic	77	$2HBr(a) = Br_2(a) + H_2(g)$
		Thermal	77	$Br_2 (l) + SO_2(g) + 2H_2O(l) = 2HBr(g) + H_2SO_4(a)$
2	UT-3 Univ. of Tokyo [4]	Thermal	600	$2Br_2(g) + 2CaO = 2CaBr_2 + O_2(g)$
		Thermal	600	$3FeBr_2 + 4H_2O = Fe_3O_4 + 6HBr + H_2(g)$
		Thermal	750	$CaBr_2 + H_2O = CaO + 2HBr$
		Thermal	300	$Fe_3O_4 + 8HBr = Br_2 + 3FeBr_2 + 4H_2O$
3	GA Sulfur-Iodine [6]	Thermal	850	$2H_2SO_4(g) = 2SO_2(g) + 2H_2O(g) + O_2(g)$
		Thermal	300	$2HI = I_2(g) + H_2(g)$
		Thermal	100	$I_2 + SO_2(a) + 2H_2O = 2HI(a) + H_2SO_4(a)$
4	Julich Center EOS [7]	Thermal	800	$2Fe_3O_4 + 6FeSO_4 = 6Fe_2O_3 + 6SO_2 + O_2(g)$
		Thermal	700	$3FeO + H_2O = Fe_3O_4 + H_2(g)$
		Thermal	200	$Fe_2O_3 + SO_2 = FeO + FeSO_4$
5	Gaz de France [7]	Thermal	725	$2K + 2KOH = 2K_2O + H_2(g)$
		Thermal	825	$2K_2O = 2K + K_2O_2$
		Thermal	125	$2K_2O_2 + 2H_2O = 4KOH + O_2(g)$
6	Nickel Ferrite [8]	Thermal	800	$NiMnFe_4O_6 + 2H_2O = NiMnFe_4O_8 + 2H_2(g)$
		Thermal	800	$NiMnFe_4O_8 = NiMnFe_4O_6 + O_2(g)$
7	LASL- U [7]	Thermal	25	$3CO_2 + U_3O_8 + H_2O = 3UO_2CO_3 + H_2(g)$
		Thermal	250	$3UO_2CO_3 = 3CO_2(g) + 3UO_3$
		Thermal	700	$6UO_3(s) = 2U_3O_8(s) + O_2(g)$
8	Ispra Mark 8 [5]	Thermal	700	$3MnCl_2 + 4H_2O = Mn_3O_4 + 6HCl + H_2(g)$
		Thermal	900	$3MnO_2 = Mn_3O_4 + O_2(g)$
		Thermal	100	$4HCl + Mn_3O_4 = 2MnCl_2(a) + MnO_2 + 2H_2O$
9	Ispra Mark 6 [5]	Thermal	850	$2Cl_2(g) + 2H_2O(g) = 4HCl(g) + O_2(g)$
		Thermal	170	$2CrCl_2 + 2HCl = 2CrCl_3 + H_2(g)$
		Thermal	700	$2CrCl_3 + 2FeCl_2 = 2CrCl_2 + 2FeCl_3$
		Thermal	420	$2FeCl_3 = Cl_2(g) + 2FeCl_2$
10	Ispra Mark 3 [5]	Thermal	850	$2Cl_2(g) + 2H_2O(g) = 4HCl(g) + O_2(g)$
		Thermal	170	$2VOCl_2 + 2HCl = 2VOCl_3 + H_2(g)$
		Thermal	200	$2VOCl_3 = Cl_2(g) + 2VOCl_2$
11	Ispra CO / Mn_3O_4 [9]	Thermal	977	$6Mn_2O_3 = 4Mn_3O_4 + O_2(g)$
		Thermal	700	$C(s) + H_2O(g) = CO(g) + H_2(g)$
		Thermal	700	$CO(g) + 2Mn_3O_4 = C + 3Mn_2O_3$
12	US -Chlorine [7]	Thermal	850	$2Cl_2(g) + 2H_2O(g) = 4HCl(g) + O_2(g)$
		Thermal	200	$2CuCl + 2HCl = 2CuCl_2 + H_2(g)$
		Thermal	500	$2CuCl_2 = 2CuCl + Cl_2(g)$
13	Ispra Mark 9 [5]	Thermal	420	$2FeCl_3 = Cl_2(g) + 2FeCl_2$
		Thermal	150	$3Cl_2(g) + 2Fe_3O_4 + 12HCl = 6FeCl_3 + 6H_2O + O_2(g)$
		Thermal	650	$3FeCl_2 + 4H_2O = Fe_3O_4 + 6HCl + H_2(g)$
14	Ispra Mark 6C [5]	Thermal	850	$2Cl_2(g) + 2H_2O(g) = 4HCl(g) + O_2(g)$
		Thermal	170	$2CrCl_2 + 2HCl = 2CrCl_3 + H_2(g)$
		Thermal	700	$2CrCl_3 + 2FeCl_2 = 2CrCl_2 + 2FeCl_3$
		Thermal	500	$2CuCl_2 = 2CuCl + Cl_2(g)$
15	ANL Mg-Cl cycle [3]	Thermal	450	$MgCl_2 + H_2O = 2HCl + MgO$
		Thermal	500	$MgO + Cl_2 = MgCl_2 + \frac{1}{2}O_2$
		Electrolytic	70	$2HCl = H_2 + Cl_2$

In recent years, two-step water splitting cycles based on metal redox reactions are becoming attractive because each of these types of cycles consists of only two steps [12,13]: an endothermic reduction reaction where oxygen is produced from a metal oxide ($M_xO_y \rightarrow M_xO_{y-1} + \frac{1}{2} O_2$), and a hydrolysis reaction where hydrogen is produced ($M_xO_{y-1} + H_2O \rightarrow M_xO_y + H_2$) . In the two reactions, M denotes a metal, e.g., zinc [14], and the subscripts x and y denote the numbers of the metal and oxygen atoms in a metal oxide molecule. The temperature for the oxygen production reaction is usually in the range of 1,500-2,500C, which cannot be satisfied by Gen-IV reactors, but can be met by concentrated high temperature solar thermal energy.

Although solar thermal energy can overcome the high temperature requirement challenge of thermochemical cycles, there are still many other challenges related to the high temperature. As illustrated in Table 1, the separations of hydrogen from steam, oxygen from sulfur dioxide, and chlorine from oxygen gas, all operate at a high temperature. To provide an efficient separation, the thermodynamic transport properties must be known for high temperatures. In addition, to provide an efficient heat transfer, the heat transfer properties of the reactants and products must be known as well.

Compared with other thermochemical hydrogen production cycles, the Cu-Cl cycle has a unique advantage of using solar thermal energy. The cycle has a molten salt intermediate product of CuCl, which could either serve as heat transfer fluid or concentrated solar thermal energy storage medium. However, thermodynamic and transport properties of CuCl at high temperatures are far from sufficient and models that can be used for the prediction of the properties have rarely been reported. So this paper will study the modeling of such properties for CuCl at high temperatures. It is expected the modeling would significantly facilitate the design and operation of both nuclear and solar-based Cu-Cl cycle.

3. THERMODYNAMIC AND TRANSPORT PROPERTIES OF STATE

Accurate knowledge of transport properties of substances is essential for the optimum design of the different items of chemical process plants, for determination of intermolecular potential energy functions and for development of accurate theories of transport properties in dense fluids. The theoretical description of these phenomena constitutes that part of nonequilibrium statistical mechanics that is known as kinetic theory.

Thermophysical properties of fluids and solids in the processes will be calculated by the Chung-Lee-Starling model (CLS) [15-22]. Equations for the viscosity and the thermal conductivity are developed based on kinetic gas theories and correlated with the experimental data. The low-pressure transport properties are extended to fluids at high densities by introducing empirically correlated, density dependent functions. These correlations use an acentric factor ω, dimensionless reduced dipole moment μ_r and an empirically determined association parameter to characterize molecular structure effects of polyatomic molecules κ, the polar effect and the hydrogen bonding effect.

The dilute gas dynamic viscosity for CLS model is written as [2,3,14-23]:

$$\eta_0(T) = 26.69579 \cdot 10^{-1} \frac{\sqrt{MT}}{\Omega^{(2,2)*}\sigma^2} F_c \tag{1}$$

The factor F_c has been empirically found to be:

$$F_c = 1 - 0.2756\omega + 0.059035\mu_r^{\,4} + \kappa \tag{2}$$

For dense fluids Eq. (2) is extended to account for the effects of temperature and pressure by developing an empirically correlated function of density and temperature as shown below [2,3,18-23]:

$$\eta = \eta_k + \eta_p \tag{3}$$

$$\eta_k = \eta_0 \left(\frac{1}{G_2} + A_6 Y \right) \tag{4}$$

$$\eta_p = \left[36.344 \cdot 10^{-6} - (MT_c)^{1/2} / V_C^{\,2/3} \right] A_7 Y^2 G_2 \exp(A_8 + A_9 / T^* + A_{10} / T^{*2}) \tag{5}$$

$$Y = \rho V_c / 6, \quad G_1 = \frac{1.0 - 0.5Y}{(1.0 - Y)^3} \tag{6}$$

$$T_c = \frac{1.2593\varepsilon}{k}, \; V_c = (0.809\sigma)^3 \tag{7}$$

$$G_2 = \frac{\{A_1(1 - exp(-A_4 Y)) + A_2 G_1 \, exp(A_5 Y) + A_3 G_1\}}{(A_1 A_4 + A_2 + A_3)} \tag{8}$$

The constants A_1-A_{10} are linear functions of acentric factor, reduced dipole moment and the association factor:

$$A_i = a_0(i) + a_1(i)\omega + a_2(i)\mu_r{}^4 + a_3(i)\kappa, i=1,10 \tag{9}$$

where the coefficients a_0, a_1, a_2 and a_3 are presented in the Table 4.

Table 4. The coefficients needed for calculation of Eq. (9)

i	a_0(i)	a_1(i)	a_2(i)	a_3(i)
1	6.32402	50.41190	-51.68010	1189.02
2	$0.12102 \cdot 10^{-2}$	$-0.11536 \cdot 10^{-2}$	$-0.62571 \cdot 10^{-2}$	$0.37283 \cdot 10^{-1}$
3	5.28346	254.209	-168.481	3898.27
4	6.62263	38.0957	-8.46414	31.4178
5	19.74540	7.63034	-14.35440	31.5267
6	-1.89992	-12.53670	+4.98529	-18.1507
7	24.27450	3.44945	-11.29130	69.34660
8	0.79716	.111764	$+0.12348 \cdot 10^{-1}$	-4.11661
9	-0.23816	$0.67695 \cdot 10^{-1}$	-0.81630	4.02528
10	$0.68629 \cdot 10^{-1}$	0.34793	0.59256	-0.72663

The same approach was employed to develop an expression for thermal conductivity:

$$\lambda = \lambda_k + \lambda_p \tag{10}$$

where:

$$\lambda_k = \lambda_0 \left(\frac{1}{H_2} + B_6 Y \right) \tag{11}$$

The thermal conductivity in the region of dilute gases for CLS model is written as:

$$\lambda_0 = 3119.41 \left(\frac{\eta_0}{M} \right) \psi \tag{12}$$

where ψ represents the influence of polyatomic energy contributions to the thermal conductivity. We used the Taxman theory [2,3,22-24] which solved the problem of influence of internal degrees of freedom on the basis of WCUB theory [8] and the approximations given by Mason and Monschick [22]. The presented expression is more accurate than the Eucken correction and the equation is supported with theory. The final expression for the influence of internal degrees of freedom is represented as:

$$\psi = 1 + C^*_{int} \left\{ \frac{0.2665 + \dfrac{(0.215 - 1.061\beta)}{Z_{coll}} + 0.28288 \dfrac{C^*_{int}}{Z_{coll}}}{\beta + \dfrac{0.6366}{Z_{coll}} + \dfrac{1.061\beta C^*_{int}}{Z_{coll}}} \right\} \tag{13}$$

where C^*_{int} is the reduced internal heat capacity at constant volume, β is diffusion term and Z_{coll} is the collision number, and is defined as the number of collisions required to interchange a quantum of internal energy with translational energy. In the presented paper we used the correlation of Z_{coll} developed by Chung, Leee and Starling [8]:

$$Z_{coll} = 2.0 + 10.5\frac{T}{T_c} \tag{14}$$

The heat capacities of ideal gases are calculated by use of statistical thermodynamics. The paper features all important contributions (translation, rotation, internal rotation, vibration, intermolecular potential energy and influence of electron and nuclei excitation). The transport term β is used to obtain the ratio between viscosity and the product between self-diffusivity at dilute gas conditions and density and shear viscosity. In our case we have used the correlation function obtained on the basis of the Pitzer acentric factor ω:

$$\beta = 0.786231 - 0.710907\omega + 1.31583\omega^2 \tag{15}$$

The residual part λ_p to the thermal conductivity can be represented with the following equation

$$\lambda_p = \left(0.1272\left(\frac{T_c}{M}\right)^{1/2}\frac{1}{V_c^{2/3}}\right)B_7Y^2H_2\left(\frac{T}{T_c}\right)^{1/2} \tag{16}$$

where λ_p is in W/mK.

$$H_2 = \left\{B_1\left[1 - exp\left(-B_4Y\right)\right]\frac{1}{Y} + B_2G_1\,exp\left(B_5Y\right) + B_3G_1\right\}\frac{1}{B_1B_4 + B_2 + B_3} \tag{17}$$

The constants B_1-B_7 are linear functions of acentric factor, reduced dipole moment and the association factor:

$$B_i = b_0(i) + b_1(i)\omega + b_2(i)\mu_r{}^4 + b_3(i)\kappa\text{, i=1, 10} \tag{18}$$

where the coefficients b_0, b_1, b_2 and b_3 are presented in Table 5.

Table 5. The coefficients needed for calculation of Eq. (18)

i	b_0(i)	b_1(i)	b_2(i)	b_3(i)
1	2.41657	0.7824	-0.91858	121.721
2	-0.50924	-1.50936	-49.9912	69.9834
3	6,61069	5.62073	64.75990	27.0389
4	14.54250	-8.91387	-5.63794	74.3435
5	0.79274	0.82019	-0.69369	6.31734
6	-5.86340	12.8005	9.58926	-65.5292
7	81.171	114.158	-60.841	466.775

4. RESULTS AND DISCUSSION

In this section, the results of the thermodynamic property evaluations will be performed over a range of temperatures. Based on the three forms of CuCl identified by Mathias [24], a step change in predicted enthalpy can be observed in the literature [24-26]. All three forms of CuCl were studied to determine the thermodynamically preferred form. In Fig. 2, the predicted enthalpy of CuCl in the liquid and gas regions is shown. A step change is observed at the phase transition point. Additional results of entropy at varying temperatures are shown in Fig. 3. In the previous results, the calculations of thermodynamic properties for solids are determined based on the following Shomate equation:

$$C_p = A + BT + CT^2 + DT^3 + \frac{E}{T^2} \tag{19}$$

$$H = \int C_p dT,\quad S = \int C_p \frac{dT}{T} \tag{20}$$

Previous studies [5] have shown that CuCl exists in two crystalline forms: a cubic form up to 412 °C and a beta-hexagonal form above this temperature. The melting point of CuCl is 423 °C, so the temperature range of the beta-hexagonal form is small. CuCl may have one of the following three preferred forms at any given temperature: CuCl (liquid), CuCl (SC) (cubic) and CuCl(SB) (beta-hexagonal). It is known that the enthalpy and the Gibbs energy of formation of CuCl(SC) at 25 °C are -137.0 kJ/mol and -120.0 kJ/mol, respectively. The enthalpy change for transition between the cubic and beta-hexagonal forms at 412 °C is 6.0 kJ/mol. Also, the enthalpy of fusion for transition from the beta-hexagonal solid to the melt at 423 °C is 7.08 kJ/mol. Using these properties, thermodynamic correlations for the three forms of CuCl can be developed and the results are shown in Figs. 2-3. The values of Gibbs free energy and enthalpy of the cubic form at 25 °C are -120 and -137 kJ/mol, respectively, since this is the stable form, at that temperature. The values G and H of the other two forms at 25 °C are set to obtain the correct enthalpy of transition and continuity in value of G. The standard-state values of G and H of the beta-hexagonal form can be obtained from the value of 6.5 kJ/mol for the enthalpy of transition from the cubic form at 412 °C.

Figure 4 shows the viscosity for molten CuCl as the comparison between model data published in article [26]. The model for viscosity was developed with statistical thermodynamics and kinetic theory. The volume for molten salt CuCl was developed from the literature [27]. Figure 5 shows the thermal conductivity of molten salt CuCl and the comparison between data published in reference [25], model developed in reference [26] and new developed CLS model. The comparison for thermal conductivity shows analytical results where thermal conductivity is around 0.3 W/mK for molten CuCl.

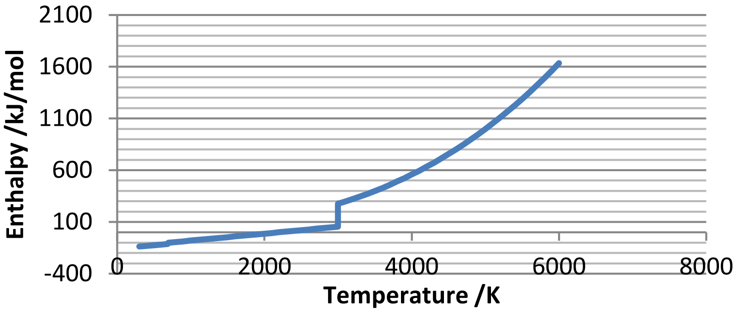

Figure 2: Enthalpy of CuCl (based on Shomate's equation)

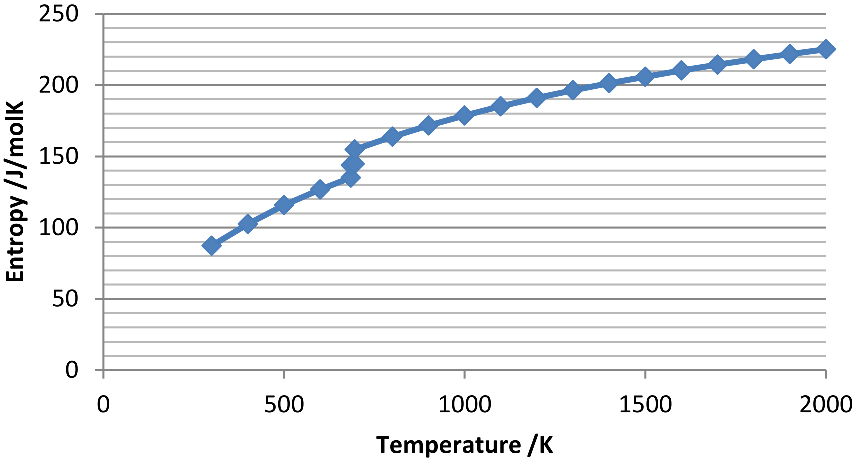

Figure 3: Entropy of CuCl (based on Shomate's equation)

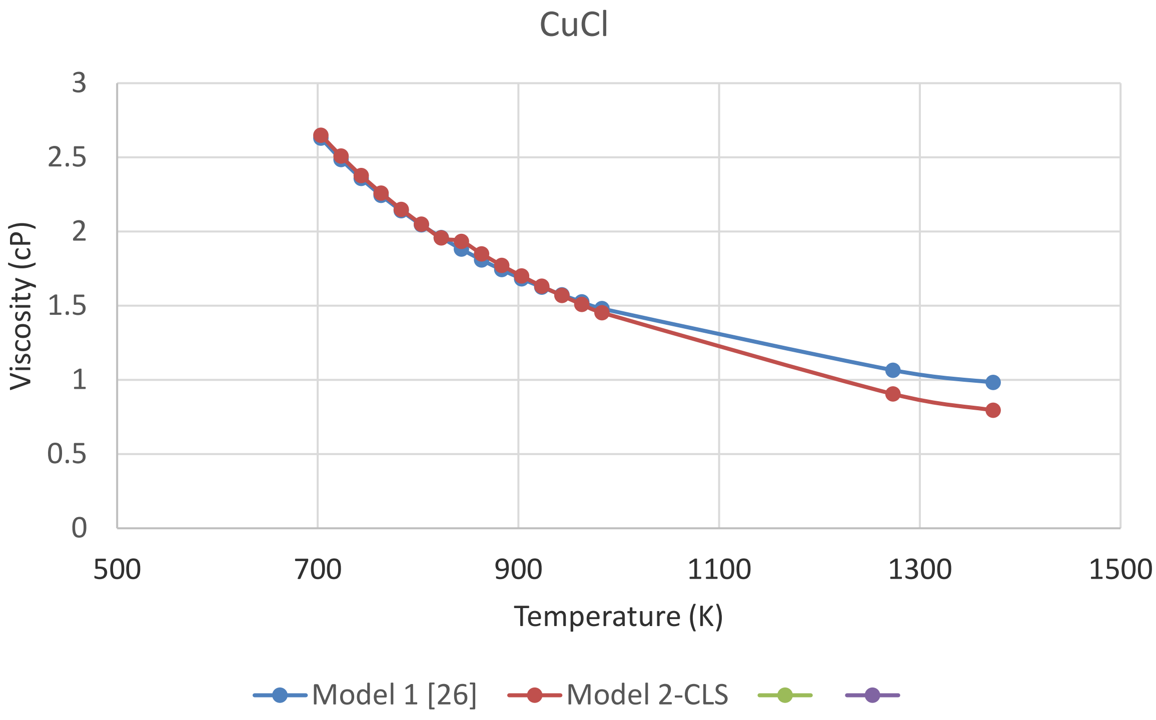

Figure 4: Viscosity for molten CuCl developed with CLS model

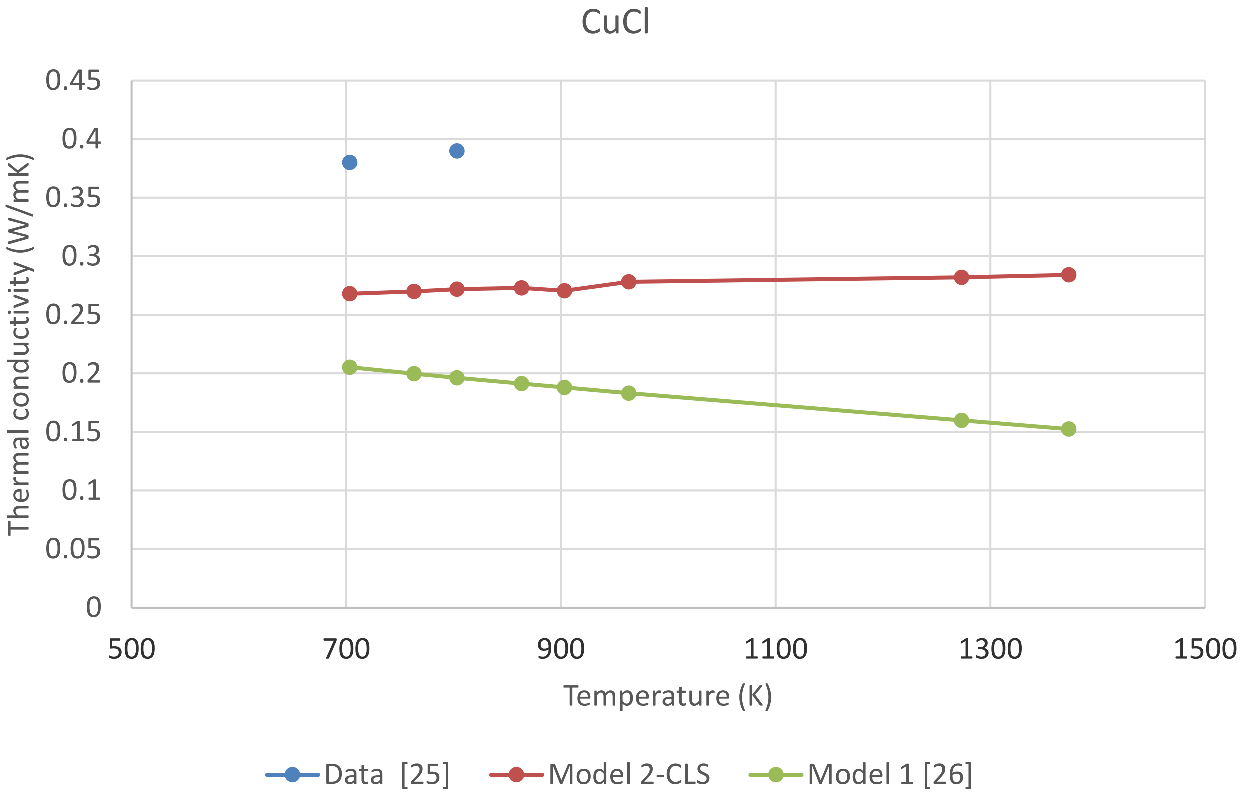

Figure 5: Thermal conductivity of molten CuCl

REFERENCES

[1] Rosen, M. A., Naterer, G. F., Sadhankar, R., Suppiah, S. Nuclear-Based Hydrogen Production with a Thermochemical Copper-Chlorine Cycle and Supercritical Water Reactor”, Canadian Hydrogen Association Workshop, Montreal, 2006, Quebec.

[2] Liu, Z. P., Li, Y. G., Lu, J. F.: *Fluid Phase Equilibria*, 2000, 173, 189-20.

[3] Petri M. C., Klickman A. E., Hori M. Hydrogen production options for water-cooled nuclear power plants. International Conference on Non-Electric Applications of Nuclear Power, 2007, Oarai, Japan.

[4] Yoshida K., Kameyama H., Aochi T., Nobue M., Aihara M., Amir R., Kondo H., Sato T., Tadokoro Y., Yamaguchi T., Sakai N. A simulation study of the UT-3 thermochemical hydrogen production process,” Int. J. Hydrogen Energy 1990 15, 171–8.

[5] Beghi G.E. A decade of research on thermochemical hydrogen at the joint research center, Ispra., International Journal of Hydrogen Energy. 1986, 11, 761–10.

[6] Besenbruch G.E. General atomic sulfur-iodine thermochemical water-splitting process. American Chemical Society, Division of Petroleum Chemistry, Preprints. 1982, 271, 48–53.

[7] Williams L.O. Hydrogen Power : an introduction to hydrogen energy and its applications. Pergamon Press. 1980.

[8] Tamaura Y., Steinfeld A., Kuhn P., Ehrensberger K. Production of solar hydrogen by a novel, 2-step, water-splitting thermochemical cycle. 1995, 20, 325–5.

[9] Bamberger C.E. Hydrogen production from water by thermochemical cycles: a 1977 update.

[10] Sadhankar R. R, Li J.; Li H.; Ryland, D. & Suppiah, S. (October 2005). Hydrogen Generation Using High-temperature Nuclear Reactors. *55th Canadian Chemical Engineering Conference*, Toronto, Canada.

[11] WNA (World Nuclear Association). Generation IV Nuclear Reactors. (accessed on June 7, 2015) Available from http://www.world-nuclear.org/info/Nuclear-Fuel-Cycle/Power-Reactors/Generation-IV-Nuclear-Reactors

[12] Xiao L., Wu S.Y. and Li Y.R. (2012) Advances in solar hydrogen production via two-step water-splitting thermochemical cycles based on metal redox reactions. *Renewable Energy*, 41, 1-12

[13] Le Gal A., Abanades S. and Flamant, G. Development of mixed metal oxides for thermochemical hydrogen production from solar water-splitting. *Parallel Sessions Book 2: Hydrogen Production Technologies - Part 1. Proceedings of the WHEC.*, 2010, 18th World Hydrogen Energy Conference 2010 – WHEC, May 16-21, 2010, Essen, Germany.

[14] Haltiwanger J. F., Davidson J. H. and Wilson E. J. Renewable hydrogen from the Zn/ZnO solar thermo chemical cycle: A cost and policy analysis. *Journal of Solar Energy Engineering*, 2010, 132, 041011-8.

[15] Avsec J., Watanabe K**.,** An approach to calculate thermodynamic properties of mixtures including propane, n-butane and isobutane. *Int. J. Thermophys.*, 2005, 6, 1769-11.

[16] Avsec J., Oblak M. Thermal vibrational analysis for simply supported beam and clamped beam. *J. Sound Vib.*, 2007, 308, 514-12.

[17] Avsec, J., Marčič, M. Calculation of elastic modulus and other thermophysical properties for molecular crystals. *J. Thermophys. Heat Transf.*, 2002, 16, 463-5.

[18] Chung, T.-H., Lee, L.L., Starling, K.E., Applications of Kinetic gas Theories and Multiparameter Correlation for Prediction of Dillute Gas Viscosity and Thermal Conductivity, Ind. Eng. Chem. Res., Vol. 27, No. 4, 1988, pp. 671-659.

[19] Chung, T.-H., Ajlan, M., Lee, L.L., Starling, K.E., Generalized Multiparameter Correlation for Nonpolar and Polar Fluid Transport properties, Ind. Eng. Chem. Fundam., Vol. 23, No. 1, 1984, pp. 8-13. Liu, Z. P., Li, Y. G., Lu, J. F.: *Fluid Phase Equilibria*, 2000, 173, 189-20.

[20] Ferziger J.H., Kasper H.G., “Mathematical Theory of Transport Processes in Gasses”, North-Holland Publishing Company, 1972, London.

[21] Avsec J., Naterer G. F., Marčič M. Non-equilibrium statistical mechanics formulation of thermal transport properties for binary and ternary gas mixtures. *Archives of Thermodynamics*, , 2008, 29, 21-15.

[22] Avsec J., "Calculation of Transport Coefficients of R-32 and R-125 with the methods of Statistical Thermodynamics and Kinetic Theories of Gas", Archives of Thermodynamics, 24, 2008, 69-13.

[23] Avsec J., Marčič, M., Influence of Multipolar and Induction Interactions on the Speed of Sound. *J. thermophys. heat transf.*, 2000, 14, 496-7.

[24] Mathias, P. M. Modeling of the Copper Chloride Thermochemical Cycle: Thermodynamic Properties of CuCl”, Technical Report, Argonne National Laboratory, USA, December 6, 2006.

[25] Liu, Z. P., Li, Y. G., Lu, J. F.: *Fluid Phase Equilibria*, 2000, 173, 189-20.

[25] Jaber, O., Heat and Fluid Flow Analysis in a Molten CuCl Heat Exchanger, Master Thesis, UOIT, 2009, Oshawa, Canada.

[26] Zamfirescu,C., Dincer, I., Naterer, G.F., Thermophysical properties of copper compounds in copper-chlorine thermochemical water splitting

[27] Janz, G.J., Thermodynamic and Transport properties for molten salts, J. Phys. Chem. Ref. Data, 17, 1988 Suppl. 2-15.