

Theoretical Study on Mechanism for the Reaction of 2-propargyl radical (C_3H_3) with ammonia (NH_3)

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Abstract: A theoretical study of the mechanism and kinetics of the reaction of 2-propargyl radical, H_2CCCH , with ammonia, NH_3 , has been carried out by ab initio molecular orbital theory based on CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++(3df,2p) method. The potential energy surface (PES) for the $C_3H_3 + NH_3$ reaction was established, showing that the reaction has four principal entrance channels. Two H-abstraction reactions from NH_3 , leading to propyne or allene + NH_2 . The addition reactions start by formation of two intermediates $H_2CCCHNH_3$ and $H_2CC(NH_3)CH$. From these two intermediate states, many other transition states and intermediate states can be accessed, leading to 21 possible products. The reaction has sizable entrance energy barriers, though the H-abstraction entrance channels might contribute significantly at high temperatures, where formation of $HCCCH_3 + NH_2$ is more energetically favorable.

Keywords: Reaction mechanism, propargyl radical, ammonia, DFT, PES.

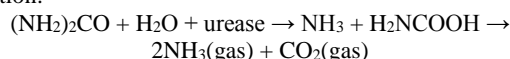
1. INTRODUCTION

Free radicals exhibit high chemical reactivity and diversities. They can react with atoms, molecules or other radicals. Propargyl (C_3H_3) is a free radical reserved much concern over the last two decades. It is known to play an important role in chemistry due to the following reasons: i) it is the first chemical species containing three carbon atoms found in interstellar medium. ii) It is an important intermediate in combustion processes. For example, it occurs with relatively significant concentration in the flames of acetylene, butadiene and benzene as well as in the decompositions of hydrocarbons in mass spectrometry.[1-3] iii) It is also the most important precursor in the formation of single and polycyclic aromatic hydrocarbons (PAHs) as well as of soot particles. For example, the recombination reaction of two propargyl radicals to yield benzene or phenyl radical (C_6H_5) which are viewed as fundamental molecules to form PAHs and soot. As small aromatic radicals such as phenyl, phenylvinyl ($C_6H_5C_2H_2$), naphthyl ($C_{10}H_7$), and their derivatives are believed to play a pivotal role in the formation of naphthalene ($C_{10}H_8$) by HACA (H-abstraction, C_2H_2 -addition) reactions and cyclization reactions. The repetition of such a successive abstraction/addition/ cyclization process involving increasingly larger aromatic radicals has been proposed as a possible route to the formation of PAHs which give rise to soot.^{2,3} iv) It also takes part in the chemical changing process of oxides of nitrogen (NO_x) and carbon (CO_x) quickly and effectively.³ The high reactivity of C_3H_3 allows it to react with species which have sustainable closed shell such as H_2O , CO , CO_2 , NH_3 , and so on.[4,5]

The formation of C_3H_3 has been clarified by many previous theoretical and experimental works.²⁻⁷ There have been investigations, both theoretically and experimentally, about the reaction of propargyl radical with other species in the interstellar medium and in combustion systems, including the self-reaction with another propargyl radical, with elements such as H, O(³P), C(³P), or with other hydrocarbon radicals such as CH_3 .⁸⁻¹³ The mechanisms of

reactions between propargyl radical with O_2 , H_2O , NO , CO , $HCNO$, OH , H , CH_3 , and C_3H_3 were investigated by our group using density functional theory.⁵ Reactions of propargyl radical with atoms or with other free radicals usually occur rapidly without energy barriers.²⁻⁴ In contrast, reactions of propargyl with neutral molecules usually have energy barriers.^{10,11,19}

There are two reasons why we choose the propargyl radical to study. Firstly, the reactions of propargyl with the oxides of nitrogen NO_x , which are important in processes such as thermal De NO_x (Process for reducing NO_x emission), NO_x -OUT (Process for reducing NO from fossil-fueled and waste-fueled stationary combustion sources), RAPRENO $_x$ (Rapid reduction of nitrogen oxides) and NO -reburning, are foreshadowed to be barrier-free leading to primary nitroso and nitro derivatives that further undergo a variety of transformations.⁸⁻¹² Secondly, the main reaction pathways of propargyl radical with either the hydrogen compounds or the hydrocarbons involves a hydrogen abstraction yielding C_3H_4 whose energy barrier is consistently low.^{13-14,19-25} As far as we are aware, little is actually known about the reactions of C_3H_3 with other simple molecules such as ammonia and hydrogen halides. In view of such scarcity of quantitative information, and in relation to our continuing study on the chemistry of propargyl radical, we set out to investigate the reaction of C_3H_3 with ammonia (NH_3). Because we know that gasification of solid fuels such as coal, biomass and peat results in a fuel gas containing high concentrations of NH_3 . This ammonia may give rise to high NO_x emissions when the fuel gas is burned. In addition, ammonia is also known to be released from the processes using urea in agriculture. More recently, various workers have measured the ammonia lost from urea applied to the surface of soils. Ernst and Massey (1960) shown that initial soil moisture increased process of losing NH_3 from surfaced-applied urea. The ammonia will likely escape to the atmosphere according to the following reaction:



where, Urease is a naturally occurring enzyme that catalyzes the hydrolysis of urea to unstable carbamic acid. Rapid decomposition of carbamic acid occurs without enzyme catalysis to form ammonia and carbon dioxide.^{26,27} Moreover, the environment with pH around 9.0 may cause soils around the applied urea particle to increase ammonia volatilization. The amount of ammonia volatilization depends on several environmental factors, including temperature, pH, and the soil water content.²⁸⁻³¹

In this study, we have theoretically mapped out the potential energy surface (PES) describing the $C_3H_3 + NH_3$ reacting system, in order to obtain essential information on the reaction rates and products distribution.

2. COMPUTATIONAL METHODS

We have characterized the mechanism of the reaction between C_3H_3 and NH_3 by quantum-chemical calculations based on the density functional theory (DFT) with the popular hybrid B3LYP functionals in conjunction with the dp-polarized plus diffuse functions 6-311++G(3df,2p) basis set.¹⁵⁻¹⁸ Vibrational frequencies and zero-point vibrational energies (ZPVE) corrections are obtained at the same level of theory. The stationary points were identified for local minima or transition states according to their vibrational analysis in which the reactants, intermediates, and products possessed all real frequencies, whereas a transition state and only one imaginary frequency. Transition states were then verified by IRC for the connectivity of the reactants and products.

In order to further improve the relative energies for all the species, single-point energy calculations were then computed using the coupled-cluster level of molecular orbital theory, incorporating all the single and double excitations plus perturbative corrections for the triple excitations, CCSD(T)/6-311++G(3df,2p), corrected for ZPE. Geometries of all species in this system have been optimized by means of the Gaussian 09 software package.¹⁹ The predicted full PES of the $C_3H_3 + NH_3$ system is presented in figure 1S of the Supporting Information (SI)³² and the energetically low-lying reaction paths are shown in figure 4.

3. RESULTS AND DISCUSSION

3.1 Reactivity prediction

In order to determine the dominant channels in the reaction system of C_3H_3 with NH_3 , we calculated and analyzed the energies of critical molecular orbitals (MO) which are shown in table 1.

Table 1. Energy values of HOMO and LUMO at the CCSD(T)/6-311++G(3df,2p) level

	E (HOMO) (eV)	E (LUMO) (eV)	ΔE (LUMO-HOMO) (eV)	
C_3H_3	-0.35631 (HOMO α)	0.03930 (LUMO α)	$C_3H_3(\alpha) -$ $NH_3(\alpha)$	0.46734
	-0.39201 (HOMO β)	0.04206 (LUMO β)	$C_3H_3(\beta) -$ $NH_3(\alpha)$	0.47010

NH_3	-0.42804 (HOMO α)	0.04349 (LUMO α)	$NH_3(\alpha) -$ $C_3H_3(\alpha)$	0.39980
			$NH_3(\alpha) -$ $C_3H_3(\beta)$	0.43550

Application of the frontier molecular orbital (FMO) theory to compute the energy values between the HOMO and LUMO (ΔE). The results in table 1 point out that the minimum energy value (ΔE) corresponds with the LUMO- α energy level of NH_3 and the HOMO- α energy level of C_3H_3 . Therefore, when the reaction takes place, electron density will move from C_3H_3 radical to NH_3 molecule to saturate valence state. These results are appropriate to form the sigma bonds in yielding the intermediates such as IS1 and IS5. The images of frontier orbitals are displayed in figure 1.

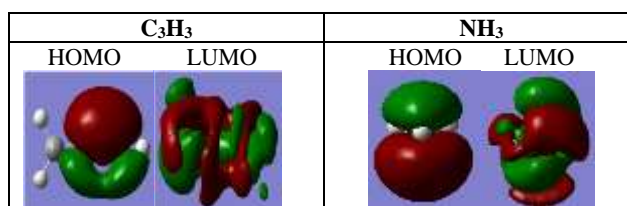


Figure 1. Images of HOMO and LUMO of C_3H_3 and NH_3

3.2 Potential energy surface and reaction mechanism

The optimized geometries of the intermediates, transition states and products at the B3LYP/6-311++G(3df,2p) level are shown in figure 2a and figure 2b. The detailed potential energy surface obtained at the UCCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) level is presented in figure 1S (see the Supporting Information), and the important reaction channels of the potential energy surface are simplified and shown in figure 3.

The scheme of the $C_3H_3 + NH_3$ reaction is presented in figure 2S of the SI. Theoretical prediction of relative energies ΔE (kcal/mol) for reactants, intermediates, transition states, and products of the reaction in different levels of theory are listed in table 2. Table 3 shows a comparison of calculated heats of reaction for the $C_3H_3 + NH_3$ system with available experimental data. In the SI, table 1S shows Gibbs free energies (ΔG) and entropies (ΔS) for different conditions, table 2S lists harmonic vibrational frequencies of the species considered, table 3S contains their cartesian coordinates and table 4S mentions theoretical predication of single point energy and ZPVE for reactants, intermediates, transition states, and products of the $C_3H_3 + NH_3$ reaction in two different levels. To help us understand the low-energy reaction pathways for the $C_3H_3 + NH_3$ system, we only concentrate on analyzing the main reaction channels illustrated in figure 3.

Table 2. Relative energies (kcal/mol) of all the stationary points considered.

Structures	B3LYP/ 6-311++G(3df,2p)	CCSD(T)/ 6-311++G(3df,2p)	Structures	B3LYP/ 6-311++G(3df,2p)	CCSD(T)/ 6-311++G(3df,2p)
C ₃ H ₃ + NH ₃ (I)	0.0	0.0	T8/P3	22.15	21.84
H ₂ CCCHNH ₂ + H (P1)	32.51	27.31	T8/12	23.65	20.93
HCCCH ₃ + NH ₂ (P2)	17.09	14.21	T4/3	34.58	34.34
H ₂ CCCH ₂ + NH ₂ (P3)	15.67	15.05	T0/P3	21.96	26.14
H ₂ CCCHNH + H ₂ (P4)	12.03	12.75	T6/7	90.00	85.57
H ₂ CCHCNH ₂ +H (P5)	49.80	42.62	T9/P6	22.84	18.71
H ₂ CCHCHNH + H (P6)	18.11	9.75	T1/4	42.51	41.99
H ₃ CCCNH ₂ +H (P7)	33.63	26.87	T1/3	39.09	37.08
CH ₃ NH ₂ +C ₂ H (P8)	62.97	56.13	T4/P6	18.39	12.98
H ₂ CCCH ₃ +NH (P9)	122.43	113.07	T3/P1	33.34	31.40
H ₂ CNH ₂ + C ₂ H ₂ (P10)	18.94	16.72	T17/P15	11.99	11.5
H ₂ CCNH + CH ₃ (P11)	4.25	4.83	T3/P4	54.94	56.91
HCCNH + CH ₄ (P12)	0.08	2.18	T3/P7	34.96	32.00
H ₃ CCN + CH ₃ (P13)	-17.8	-22.97	T1/6	94.11	93.35
C ₂ H ₄ + CNH ₂ (P14)	27.22	25.34	T7/P5	59.25	59.16
C ₂ H ₄ + HCNH (P15)	4.98	3.38	T5/8	42.73	40.06
C ₂ H ₅ + HCN (P16)	-9.8	-15.35	T4/9	21.59	19.54
C ₂ H ₅ + CNH (P17)	3.08	-1.67	T3/P2	23.36	21.63
C ₂ H ₂ +HCNH ₃ (P18)	86.21	82.24	T12/P12	87.57	87.64
H ₃ CCH ₂ CN + H (P19)	-0.13	-11.81	T4/10	34.05	34.51
cyc-HCCHNHCH ₂ +H (P20)	42.14	31.19	T10/11	49.79	45.94
HCCCH ₂ NH ₂ +H (P21)	40.12	30.27	T11/20	54.02	51.56
I1	34.69	35.51	T11/P10	28.97	28.09
I3	-3.5	-6.46	T10/P3	21.31	22.31
I4	-30.72	-31.66	T12/13	13.05	8.52
I5	40.33	37.36	T13/P13	-5.3	-10.22
I6	54.4	51.87	T4/14	36.55	35.14
I7	34.18	30.64	T16/17	14.43	12.41
I8	-27.51	-30.46	T14/P5	55.41	52.37
I9	-6.28	-11.33	T14/P14	35.49	33.53
I10	2.6	-1.73	T3/15	38.65	37.38
I11	5.39	-0.16	T3/16	31.72	30.62
I12	-27.42	-31.70	T6/P18	89.38	86.3
I13	-30.16	-35.95	T15/18	48.48	45.85
I14	20.06	15.30	T1/20	103.18	98.28
I15	-7.76	-10.89	T16/18	24	23.05
I16	-28.73	-31.45	T11/21	45.31	41.11
I17	-12.99	-18.74	T20/P21	45.43	42.25
I18	-15.36	-19.57	T18/P19	4.64	-0.70
I19	-24.88	-30.72	T17/18	24.3	21.42
I20	41.77	38.19	T21/P20	46.59	42.04
I21	43.03	37.72	T15/16	33.6	31.31
T0/5	40.29	39.62	T16/19	18.93	14.17
T0/P2	23.29	23.94	T16/18	22.09	21.15
T0/1	34.15	36.62	T19/P19	4.7	-2.24
T1/P1	39.39	41.29	T19/P16	-1.76	-6.64

(a) The addition pathways. It can be seen from figure 3, there are two addition entrance channels of the reactants. Addition of NH₃ onto C₃H₃ is possible at two carbon atoms. The attack at the central carbon, giving rise to an intermediate I₅(H₂C=C(NH₃)-CH) through TS₁, occurs without a pre-association complex and with a high energy barrier of 39.6 kcal/mol. This process is predicted to be endothermic by 37.36 kcal/mol with a tight transition state. The C-N distance in TS₁ (see in figure 2b) is quite long (1.8 Å), which is suitable with structure of a transition state. From the intermediate I₅, an isomeric intermediate I₈ (H₂C=C(NH₂)-

CH₂) was formed via a H-migration transition state TS₂₁ with the energy barrier of 2.7 kcal/mol. Conformer I₈ lies below the reactants by 30.46 kcal/mol. Once I₈ is formed, it can be converted in two ways, namely (i) a NH₂-loss giving allene (H₂C=C=CH₂) P₃ by crossing through the transition state TS₅ (shown in figure 2b) with an 21.84 kcal/mol barrier above the reactants, and (ii) a 1,7-H-shift yielding I₁₂ (H₃C-C(NH)=CH₂, -31.7 kcal/mol) via TS₆ overcoming an energy barrier of 51.39 kcal/mol. The lower TS of the two, TS₆, still lies 20.93 kcal/mol above the energy of the free reactants. The formation of the product P₃ (H₂C=C=CH₂ + NH₂) from the channel

passing through three transition states (TS₁, TS₂₁, TS₅) and two intermediate states (I₅, I₈) is endothermic by 15.05 kcal/mol. Following the formation of I₁₂, there are two reaction channels, of which one goes directly to products P₁₁ (H₂CCNH + CH₃) without an exit energy barrier, while the other takes place via transition state TS₃₁ at 8.52 kcal/mol above the reactants, forming intermediate I₁₃ (H₃C-C(N)-CH₃), which is by far the lowest-energy isomer of the PES at -35.95 kcal/mol. I₁₃, however, is relatively unstable with

respect to a C-C bond cleavage via TS₃₂ (-10.22 kcal/mol) producing P₁₃ (H₃CCN + CH₃, -22.97 kcal/mol), the lowest-lying fragment products.

The data in figure 3 shows that the energy of product P₁₃ (-22,97 kcal/mol) is lower than that of the product P₁₁ (4.83 kcal/mol) by 27.8 kcal/mol, but the pathway producing P₁₃ has to pass through many high energy barriers. Thus, the product P₁₁ is more easily formed while P₁₃ is the most stable one compared to all others of the PES.

Table 3. Comparison of Calculated Heats of Reaction for C₃H₃ + NH₃ with Experimental Data.

Species	B3LYP/6-311++G(3df,2p) (kcal/mol) ^a	CCSD(T)/6-311++G(3df,2p) (kcal/mol) ^a	Experiment (*) (kcal/mol)
H ₂ CCCHNH ₂ +H (P1)	32.15	26.95	---
HCCCH ₃ +NH ₂ (P2)	17.82	14.12	14.01±1
H ₂ CCCH ₂ +NH ₂ (P3)	15.49	14.87	15.74±1
H ₂ CCCHNH+H ₂ (P4)	12.36	12.81	---
H ₂ CCHCNH ₂ +H (P5)	49.30	42.12	---
H ₂ CCHCHNH+H (P6)	17.48	9.12	---
H ₃ CCCNH ₂ +H (P7)	33.24	26.48	---
H ₂ CNH ₂ +C ₂ H ₂ (P10)	18.56	16.34	16.93±0.2
H ₂ CCNH + CH ₃ (P11)	4.09	4.67	---
HCCNH + CH ₄ (P12)	0.04	2.14	---
H ₃ CCN + CH ₃ (P13)	-17.96	-23.13	-21.49±2
C ₂ H ₄ + CNH ₂ (P14)	26.67	24.79	---
C ₂ H ₄ + HCNH (P15)	4.42	2.82	---
C ₂ H ₅ + HCN (P16)	-10.04	-15.59	-14.91±0.7
C ₂ H ₅ +CNH (P17)	3.16	-1.59	-0.06±1.5
H ₃ CCH ₂ CN + H (P19)	-0.63	-12.30	-9.48±2
cyclo-HCCHNHCH ₂ +H (P20)	41.04	30.09	---
HCCCH ₂ NH ₂ + H (P21)	39.76	29.92	---

^a The exothermicity for the formation of C₃H₃ + NH₃ was calculated on the basis of the experimental heats of formation at 0 K, (*) from reference.¹⁹

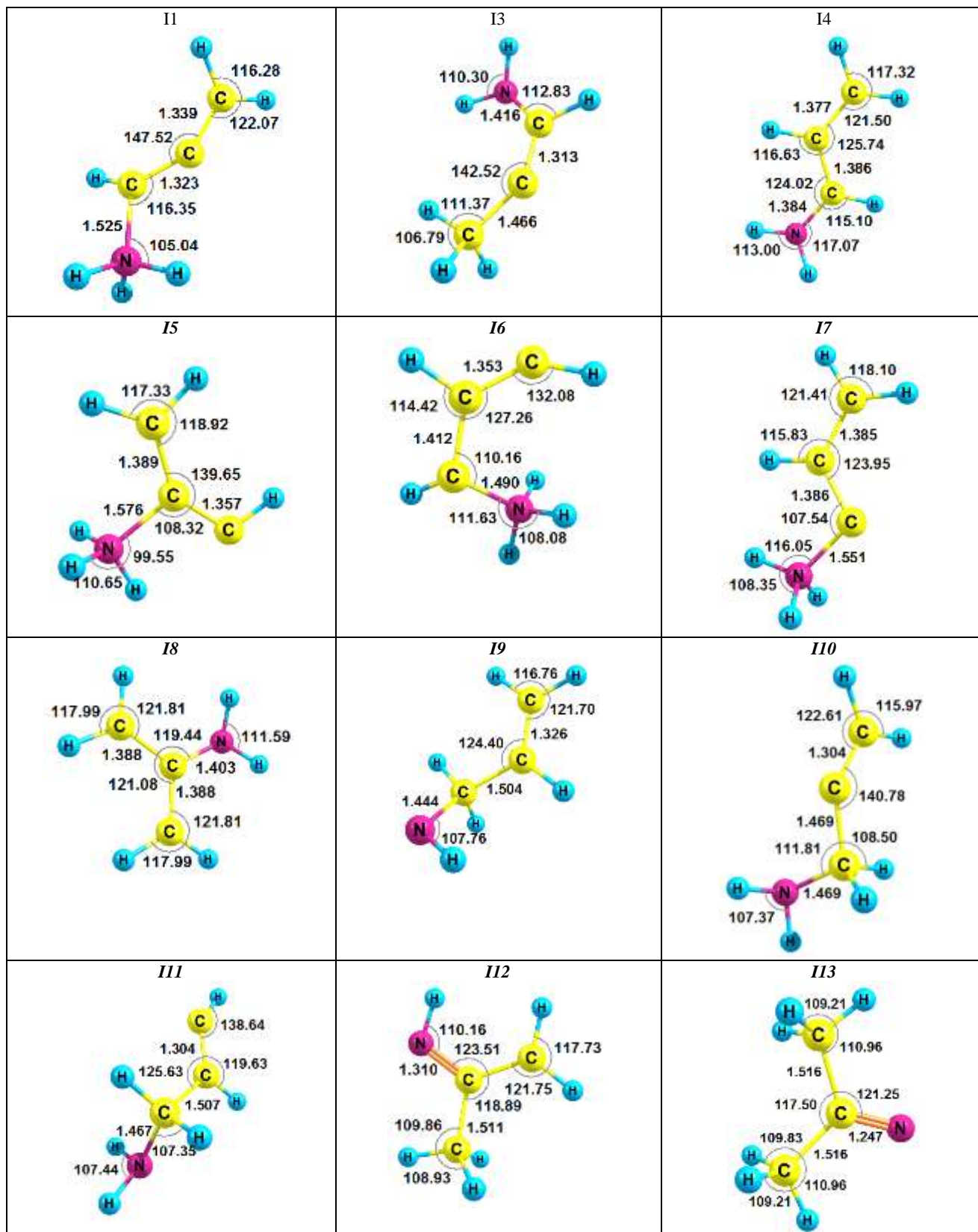
Attack on the terminal carbon of C₃H₃, is initiated by formation of a pre-reactive complex, followed by a high energy barrier TS₃ of 36.62 kcal/mol, yielding I₁ (H₂C=C-CH-NH₃, 35.51 kcal/mol). The distance of 1.63 Å for the C-N bonding TS₃ (see in Fig. 2b) is now much shorter than that in TS₁ above. In both cases of the initial addition reaction paths, the attack angle is around 105-118° and the ammonia moiety apparently exhibits a similar configuration. As shown in figure 3, the I₁ intermediate can first isomerize to I₃ (H₃C-C=CH-NH₂, - 6.46 kcal/mol) via TS₁₃ with a small 1.57 kcal/mol barrier; followed either by isomerization to the open-chain I₁₆ (H₃C-CH=CH-NH, - 31.45 kcal/mol) via the 1,4-H-shift TS₃₈ with a rather high 37.08 kcal/mol barrier, or by fragmentation to product P₂ (HCCCH₃ + NH₂) by breaking the C-N bond via TS₂₃ with a barrier of 28.09 kcal/mol. The overall exothermicity of the process leading to the product P₂ is -14.21 kcal/mol. From intermediate I₁₆, there are three other isomerization channels, leading to intermediates I₁₇ (H₂C-CH₂-CH=NH), I₁₈ (H₃C-CH₂-C=NH), and I₁₉ (H₃C-CH₂-CH=N) with isomerization barriers of 43.86, 52.6, and 45.62 kcal/mol, respectively. A 1,4-H shift connects I₁₇ and I₁₈ with the energy barrier via TS₄₇ of 40.16 kcal/mol, where the angle N-C-C changes slightly from 123° in I₁₇ to 137° in I₁₈. I₁₇ fragmentation over the 30.24 kcal/mol barrier height of TS₁₆ produces product P₁₅ (C₂H₄ + HCNH) with 3.38 kcal/mol of endothermicity. In figure 3, one sees that product P₁₉ (H₃C-

CH₂-CN + H) can be formed in two ways; one taking place via the intermediate I₁₈, while the other via the intermediate I₁₉. The energy of the transition state TS₅₄ in the first path is lower than that of TS₄₆ in the latter by only 1.54 kcal/mol. Furthermore, two products, namely P₁₆ (C₂H₅ + HCN) and P₁₇ (C₂H₅ + CNH), can also form from I₁₉ and I₁₈, respectively. P₁₇ was produced directly from I₁₈ without any exit energy barrier, whereas the product P₁₆ was produced by the C-C bond-breaking process with an energy barrier of 6.46 kcal/mol below the entrance point. It is clear that product P₁₆ is more stable than product P₁₇. Formation of both of these is exothermic with relative energies of -15.35 kcal/mol and -1.67 kcal/mol, respectively. The I₁ intermediate formed in the current addition reaction can also undergo isomerization to another isomer I₄ (H₂C=CH-CH-NH₂, -31.66 kcal/mol,) via TS₁₂ with a 6.48 kcal/mol barrier. This barrier is higher than that of the earlier process forming the isomer I₃ with only 1.57 kcal/mol barrier height. This latter path is therefore expected to contribute less significantly. The I₄ intermediate further dissociates to product P₆ (H₂CCHCHNH + H) via TS₁₄ with a 12.98 kcal/mol barrier above the reactants. I₄ can also isomerize to I₉ (H₂C=CH-CH₂-NH, -11.33 kcal/mol) by a 1,7-H shift via TS₂₂ with 19.54 kcal/mol above the entry point, and then breaking the C-H bond in I₉ forming the same product P₆ via TS₁₁ costing 30.04 kcal/mol energy. The isomerization transition state (TS₇) between I₄ and I₃ is also

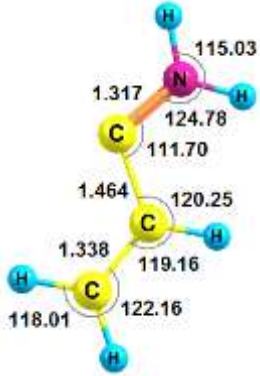
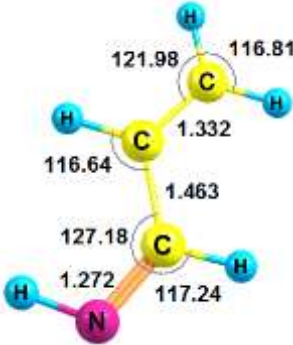
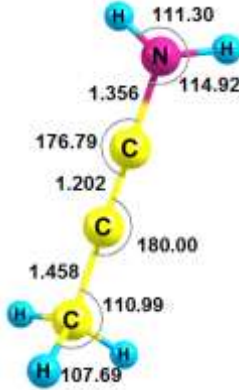
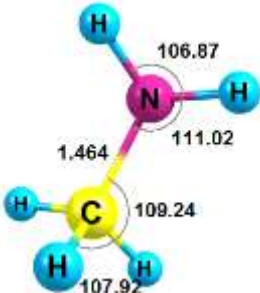
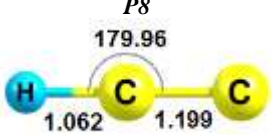
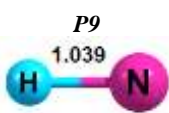
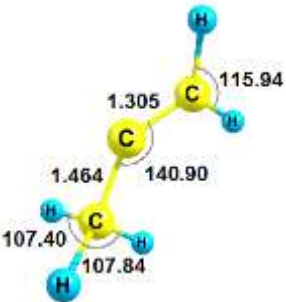

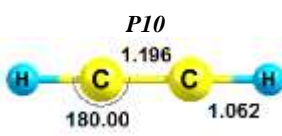
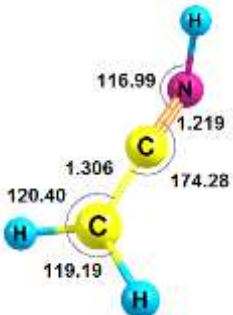
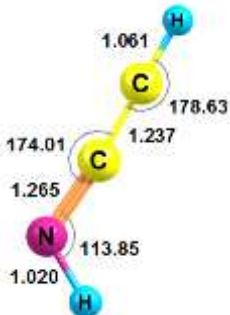
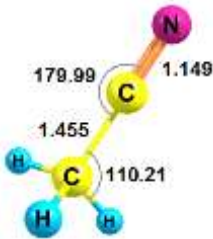
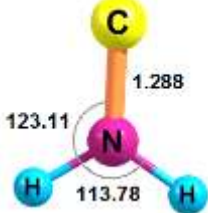
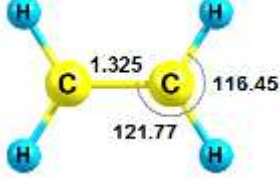
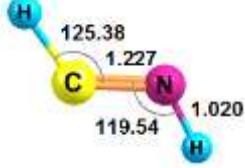
located; its energy is 34.34 kcal/mol higher than that of the reactants.

We can see that both of the addition pathways illustrated in figure 3 can produce many different products. The entrance transition structure, TS₁ (39.62 kcal/mol), is found to be higher in energy than TS₃ (36.62 kcal/mol); accordingly, it is

concluded that the latter pathway takes place relatively faster than the former. As both these transition states are high in energy, all products formation through these two channels is controlled mainly by TS₁ and TS₃, and is expected to be kinetically unfavorable.



<p>I14</p>	<p>I15</p>	<p>I16</p>
<p>I17</p>	<p>I18</p>	<p>I19</p>
<p>I20</p>	<p>I21</p>	<p>P1</p>
<p>P2</p>	<p>P3</p>	<p>P4</p>
<p>P5</p>	<p>P6</p>	<p>P7</p>

		
<p><i>P8</i></p> 	<p><i>P8</i></p> 	<p><i>P9</i></p> 
<p><i>P9</i></p> 	<p><i>P10</i></p> 	<p><i>P10</i></p> 
<p><i>P11</i></p> 	<p><i>P12</i></p> 	<p><i>P13</i></p> 
<p><i>P14</i></p> 	<p><i>P14</i></p> 	<p><i>P15</i></p> 
<p><i>P16</i></p>	<p><i>P17</i></p>	<p><i>P18</i></p>

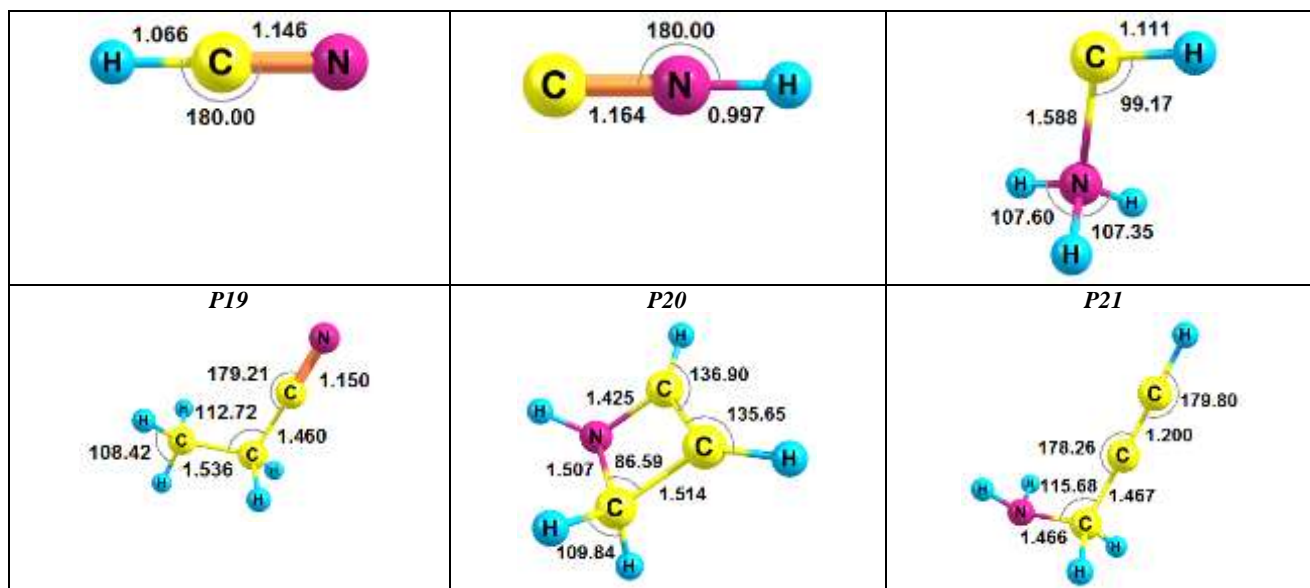
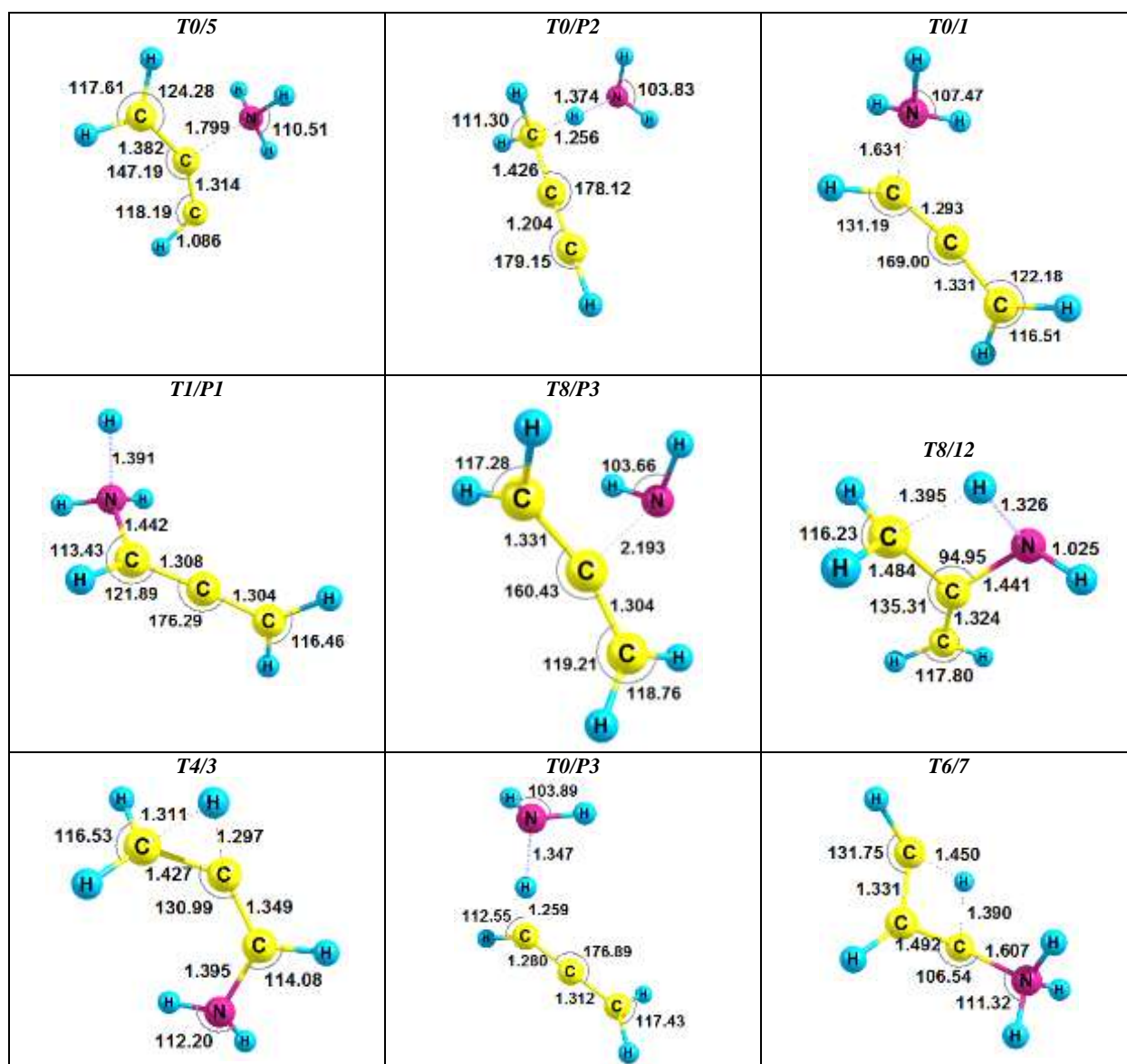


Figure 2a. Optimized geometries of the intermediate states and products involved in the reaction of $C_3H_3 + NH_3$ at the B3LYP/6-311++G(3df,2p) level. (The bond lengths are given in angstroms and angles in degrees).



<p><i>T9/P6</i></p>	<p><i>T14</i></p>	<p><i>T1/3</i></p>
<p><i>T4/P6</i></p>	<p><i>T3/P1</i></p>	<p><i>T17/P15</i></p>
<p><i>T3/P4</i></p>	<p><i>T3/P7</i></p>	<p><i>T1/6</i></p>
<p><i>T7/P5</i></p>	<p><i>T5/8</i></p>	<p><i>T4/9</i></p>
<p><i>T3/P2</i></p>	<p><i>T12/P12</i></p>	<p><i>T4/10</i></p>

<p><i>T10/I1</i></p>	<p><i>T11/I20</i></p>	<p><i>T11/P10</i></p>
<p><i>T10/P3</i></p>	<p><i>T12/I3</i></p>	<p><i>T13/P13</i></p>
<p><i>T4/I4</i></p>	<p><i>T16/I7</i></p>	<p><i>T14/P5</i></p>
<p><i>T14/P14</i></p>	<p><i>T3/I5</i></p>	<p><i>T3/I6</i></p>
<p><i>T6/P18</i></p>	<p><i>T15/I8</i></p>	<p><i>T1/I20</i></p>

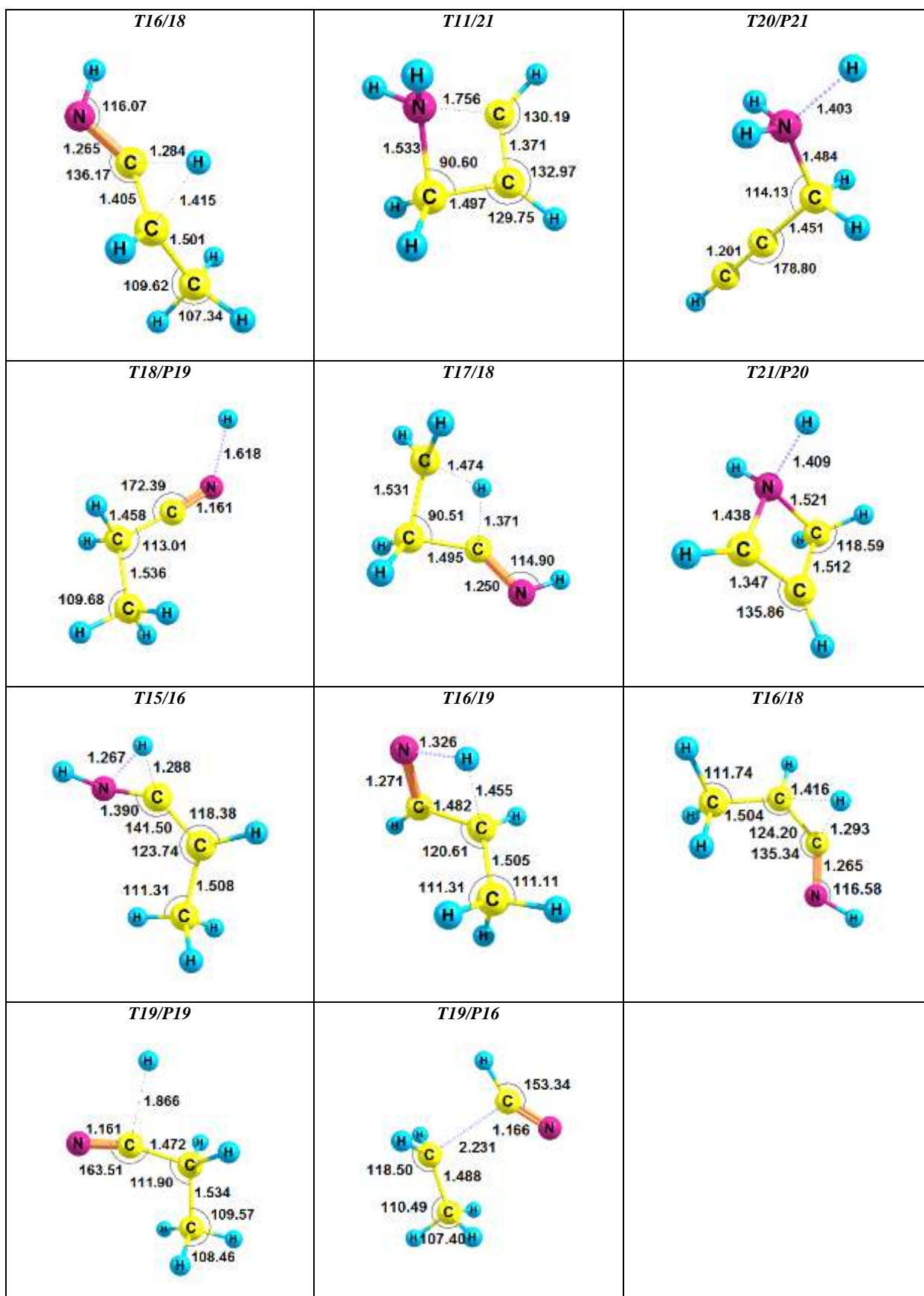


Figure 2b. Optimized geometries of the transition states involved in the reaction of $C_3H_3 + NH_3$ at the B3LYP/6-311++G(3df,2p) level. (The bond lengths are given in angstroms and angles in degrees).

(b) The hydrogen abstraction pathway. The figure 4 shows that H-abstraction takes place in two channels. The first abstraction channel creates P₂ via only one transition state TS₂ with an energy barrier of 23.94 kcal/mol. Although not having a pre-reactive complex at the beginning of this pathway, the products are formed in a complex with a relative energy value of 12.39 kcal/mol above the energy of the free reactants, before separating without an exit barrier. In the structure of TS₂ (see in figure 2b), when the molecular ammonia approaches the propargyl radical, one of three hydrogen atoms abstracts from ammonia at the distance of 1.374 Å to bond with the carbon atom at the distance of 1.256 Å. In this case, the bond lengths of N...H and C...H are longer than the experimental bond lengths of them³³ about 0.355 and 0.166 Å, respectively. The latter is slightly stable with respect to the separated fragments P₂ (HCCCH₃ + NH₂, 14.21 kcal/mol). The distance between H and N in the Com1 is elongated by 1.459 Å when going from the TS₂ to Com1. The complex further dissociates to P₂ without transition state. Moreover, it is easy to realize that, the product P₂ is also produced by the additional reaction mechanism as discussed above. Comparing these two mechanisms, one finds that,

relatively, the latter mechanism takes place more readily than the former mechanism.

Product P₃ is formed by the second abstraction channel through transition structure TS₈ (shown in Figure 2b) with an energy barrier of 26.14 kcal/mol. In the geometry of TS₈, the distances of N...H and C...H are calculated to be about 1.347 and 1.259 Å, respectively; the angle C-C-H changes by more than 61° from 180° in C₃H₃ to 128.42° in TS₈, which suggests that this transition is a critical motion in this transition state, and relates to the re-hybridisation of the carbon atom from sp to sp². Dissociation to the separated products H₂CCCH₂ + NH₂ (P₃) occurs by an extremely small dissociation energy of 0.7 kcal/mol compared to the complex (H₂C=C=CH₂...NH₂, 14.35 kcal/mol). In this process there is no exit barrier for the loose bond cleavage. In the final product, the newly formed C-H bond length is shortened to 1.08 Å in H₂CCCH₂. Formation of product, H₂CCCH₂ + NH₂, is found to be endothermic by 15.05 kcal/mol at the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) level.

It is obvious that formation of product P₂ via TS₂ is more favorable than product P₃ formed through TS₈.

The results given above clearly demonstrate that the hydrogen abstraction is preferred over the additional reaction.

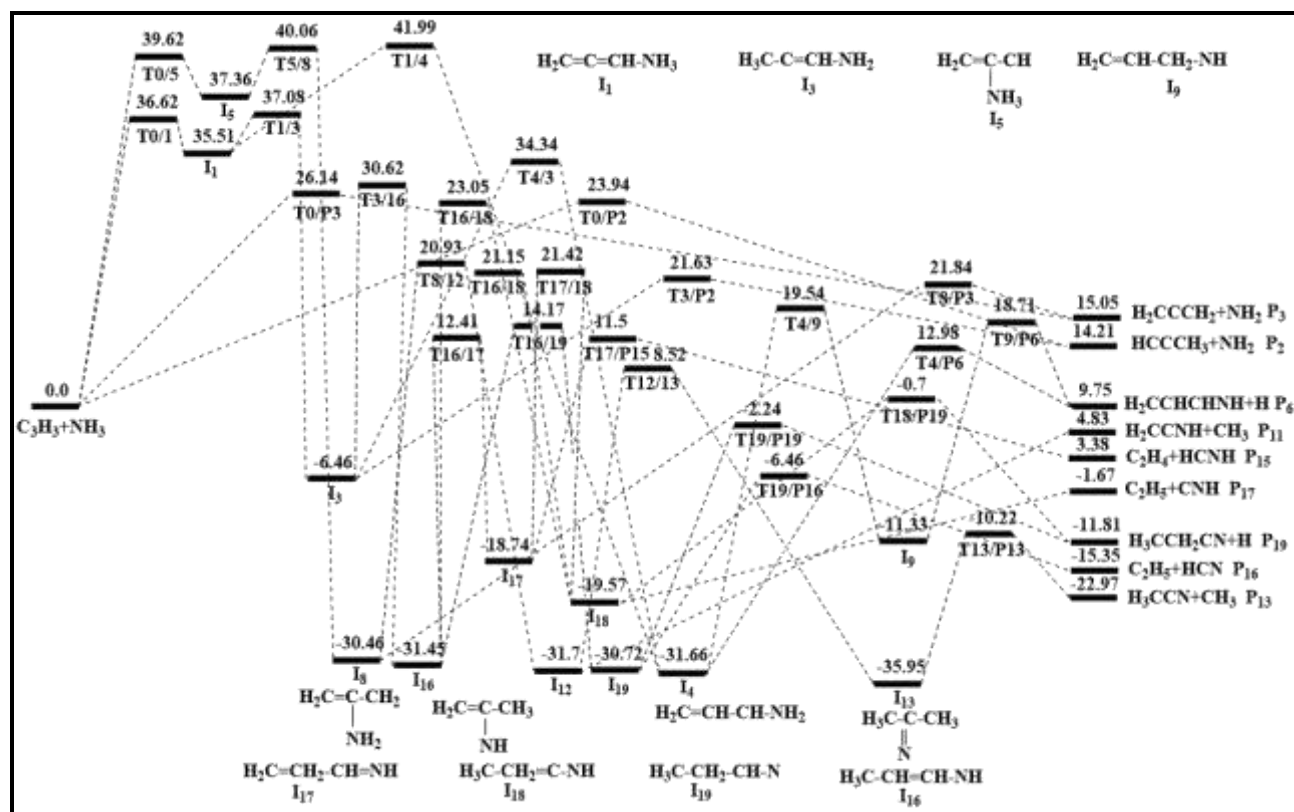


Figure 3. The simplified potential energy surface of the C₃H₃ + NH₃ reaction. Energies are in units of kcal/mol calculated at the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) + ZPVE level.

4. CONCLUSION

By application of the density functional theory, we have optimized geometric structures of reactants, intermediate substances, transition states, and products of the C₃H₃ + NH₃ reaction system, based on the CCSD(T)/6-311++G(3df,2p)//B3LYP/6-311++G(3df,2p) methods.

In the present theoretical study, we have mapped in detail the [C₃H₆N] potential energy surface, with emphasis on the

sections guiding the four main reaction routes for the C₃H₃ + NH₃ reaction, namely the hydrogen abstractions and addition reactions. Calculated results indicate that products of this reaction can be P₁ to P₂₁ as shown in the full PES. The formation of P₂ (HCCCH₃ + NH₂) is the most energetically favorable. However, the product H₃CCN + CH₃ (P₁₃) is the most stable product in energy. Calculated enthalpies of

formation for five reaction pathways P₂, P₃, P₁₀, P₁₃, P₁₆, P₁₇, and P₁₉ are in good agreement with experimental data, which suggests that the theoretical methodology is reliable.

We find that the hydrogen abstraction is expected to dominate at all temperatures. However, due to its rather lower-lying energies of products, the addition emerges as a

5. ACKNOWLEDGMENTS

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Design of Solar Panel for 1.5 Hp Nano Coated Motor Used in Ball Mills for Producing Nano Powders in Pyro Industries in Sivakasi

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Abstract: This paper deals with the design of nano coated motor used in ball mills used for producing nano powders in pyro industries in Sivakasi. This paper also briefs about the profile of industries and administration of Virudhunagar district. A brief history of Virudhunagar district was also discussed. This paper deals with the industrial application of nano coated motor used in the preparation of nano powders used in pyro industries located in Sivakasi. Design of solar panel for 1.5 Hp nano coated motor was given in nice manner for the understanding of young researchers to design the solar cells for the nano coated motor. These nano coated motors were used in pyro industries for producing nano powders in ball mills in Sivakasi.

Keywords: Solar panel, nano coated motor, pyro industries, ball mills, Sivakasi, Virudhunagar district. Enamel,

1. INTRODUCTION

This paper deals with the industrial application of nano coated motor used in the preparation of nano powders used in pyro industries located in Sivakasi. Particle sizes of powders used in pyro industries were in nano size. So, pyro industries were called as Nano pyro industries. Balls mills were used to produce Nano pyro powders. Induction motors were used in Ball mills. Nano coated windings were used in Induction motor and hence, these motors were called as nano coated induction motors. These nano coated induction motors were operated by solar power. Hence, these kinds of motors were called as solar power operated Nano coated induction motor. These motors can be used in ball mills to produce nano pyro powders in pyro industries in Sivakasi. Hence the article was

named as “Solar power operated Nano coated Induction motor used in Ball mills in Nano pyro industries in Sivakasi”.

Sivakasi was a mega industrial hub in Virudhunagar district. Virudhunagar district was carved on 15th March 1985 by trifurcation of the composite Ramanathapuram district with head quarters at Virudhunagar. The district lies between 55.00 Degree and 77.00 Degree of the eastern longitude and between 9.00 Degree and 55.00 Degree of the northern latitude. It has an area of 4243 Sq Km and is bounded on the west by Kerala State, on the north by Madurai and Sivaganga district, on the east by New Ramanathapuram district and on the south by Tirunelveli and Tuticorin districts.

Virudunagar is a small town located at a distance of 45 Kms South-West of Madurai. This place was once referred to as

'Virudupatti'. In the beginning of 20th century A.D., Virudupatti was one among the six important places of Ramanathapuram District. Due to the rapid growth in the field of Trade and Education, it was renamed as 'Virudunagar' on 29th October 1923. The term 'virudu' means 'Award' in Tamil. The people of this community migrated to improve their business status and settled in Virudunagar during 19th century A.D. Virudunagar exports all kinds of oil to Dubai and Srilanka and also exports Cotton, chilli, spices, cardamom to USA and Singapore. Virudunagar is a famous business centre without markets. The Business people of Virudunagar play an important role in price fixation of consumer products. Hence there is a popular saying, "virudunagar produces nothing but controls everything".

In 1985, the erstwhile Ramanathapuram District was trifurcated to create the districts of Ramanathapuram, Pasumpon Muthuramalinga Thevar Tirumagan (later renamed Sivaganga) and Kamarajar District (later renamed Virudhunagar District).

The District headquarters is Virudhunagar town. It covers an area of 4232 sq. km and is divided into 8 taluks, namely Aruppukkottai, Kariapatti, Rajapalayam, Sattur, Sivakasi, Srivilliputtur, Tiruchuli and Virudhunagar. On 3rd March 1996, Sivakasi taluk was created separating the firkas of Sivakasi, Edirkottai and Salwarpatti from Sattur taluk and Mangalam firka from Virudhunagar taluk. In 31st August 1998, Kariapatti taluk was formed by separating Kariapatti, Mudukkankulam and Kalkurichi firkas from Aruppukkottai taluk. Mallanginar firka, the 4th firka of the taluk was carved out of Kalkurichi firka. The District is divided into two Revenue Divisions comprising four taluks each. The Aruppukkottai Revenue Division comprises Kariapatti, Tiruchuli, Aruppukkottai and Virudhunagar taluks, and Sivakasi Revenue Division of Sattur, Sivakasi, Srivilliputtur and Rajapalayam taluks.

According to the 2011 census Virudhunagar district has a population of 1,943,309, roughly equal to the nation of Lesotho or the US state of West

Virginia. This gives it a ranking of 242nd in India (out of a total of 640). The district has a population density of 454 inhabitants per square kilometre (1,180 /sq mi). Its population growth rate over the decade 2001 - 2011 was 10.96 %. Virudhunagar has a sex ratio of 1009 females for every 1000 males and a literacy rate of 80.75 % [2]. It is 44.39 % urbanized. Majority of the population are involved in Industries and agriculture. The total area of Virudhunagar District is 3445.73 km.

The climate is generally hot and dry with a low degree of humidity. The District receives scanty rainfall. The average annual rainfall is only 987.7 mm. The frequent drought caused by the failure of the monsoon adversely affects the dry crops depending upon rain fed tanks for irrigation. Soil is predominately black soil.

Virudhunagar has rich mineral deposits of lime kankar and granite also. The lime and limestone deposits are concentrated in Pandalkudi, Chettipatti and Velayudhapuram villages of Arupukottai taluk and Cholapuram and Perumalpatti of Rajapalayam taluk and Gopalapuram, Kangaseval and Vertrilaiyurani of Sattur taluk. Likewise, kankar deposits are found abundant in Kilavarneri and P. Pudupatti in Kariapatti blocks of Arupukottai taluk. Granite deposits are also found in

Thiruthangal in Sattur taluk and Pillaiyarkulam in Srivilliputtur taluk.

The forests are found on the eastern slopes of the Western Ghats. Only 6.3% of the total geographical area of the district is under forests. Many rare and endemic varieties of flora and fauna are found along the mountain slopes. A wildlife sanctuary, spread over 480 sq. kms was established in 1989 at Shenbagathopu in Srivilliputtur taluk. The forests of Alagarkoil valley in Srivilliputtur taluk and Saduragiri are known for rare medicinal plants. The medicinal value of 275 plants has been recorded and reported. The forests host a rich variety of orchids and ferns.

The district has got 3 revenue divisions, 7 municipalities, 11 blocks and 9 taluks respectively. The district is endowed with a semi arid tropical climate with an average rainfall of 985.7 mm. The predominant soil type is black loamy. This type of soil is found common in Sattur, Srivilliputtur, and Aruppukkottai blocks.

Existence of Industrial estate attracts investment opportunities. The Tamil Nadu Small Industries Development Corporation (SIDCO) is the agency for establishing and maintaining industrial estates for tiny and small-scale industries in this district/state. Two Industrial Estates are functioning at Virudhunagar and Rajapalayam. A Cooperative Industrial Estate is also functioning at Sivakasi. SIDCO has also constructed Tiny Industrial Sheds at Watrap, Kariapatti and Thiruchuli.

Virudhunagar district is known for concentration of multiple enterprises in different part of the district. Each block is unique in nature. Concentration industries like Match, Fireworks, Printing, Oil Extraction, readymade garments, Brick Making, Surgical cotton, textile products, cement, lime based products, rice mill, paper products, food industries, tin containers, gold jewellery making in different parts of the district the district offer multiple intervention for further development. It attracts the attention of the policy makers and reaches to anchor the industrial development in a balanced manner across the district. Cotton is a major commercial crop of the District and the cotton industry therefore occupies an important place in the economy. Rajapalayam is the chief centre for spinning mills and ginning factories. Surgical cotton and bandage cloth are manufactured here. Textile mills in the produce a variety of cotton yarn and valued added textile products. The District has huge deposits of limestone and gypsum. It paves the way to establish lime based and cement industry Tamil Nadu Cements – a Public Sector undertaking at Alangulam and Madras Cements – a Private Sector undertaking at Thulukkappatti are two large cement producing units situated in this district.

Sivakasi and Sattur are known for the match industry. There are over 4500 match unit concentrated in this district giving employment to more than lakh plus people. There are nearly 450 fireworks factories giving direct employment, to about 40,000 workers and about 1 lakhs indirect such as paper tube making, Wire cutting, Box making sale distribution in the country side. The market for fire works is likely to grow at the rate of 10% per annum. The annual output is over 50,000 tones, and turn over (at factory cost) around Rs. 350 crores according to industrial sources.

Explosives for blasting are also manufactured here. Over 70% of the total production of matches and fireworks in India is

manufacture in Virudhunagar District. A large percentage of crackers are exported. Sivakasi, renowned the world over for its printing, Litho Presses, offset printing machines of which is the second largest number in the world, next to Guthenburg, a city in Germany. Around 450 printing presses including offset & flexo types are located in and around Sivakasi.

The printing industry was originally established to supply labels for the match and firework industries. Soon the industry developed and diversified into other areas of printing like books, posters, greeting cards and diaries. Sivakasi now offers state of the art, world class printing facilities. Sattur town was once very famous for fountain pen nib manufacturing industries. More than 2000 families were involved in this industry. But during the recent times, usage of fountain pen has come down to larger extent and hence the industry is in declining trend. This industry, which was once the bread winning industry of the town has almost, vanished now.

Sundaram Fasteners and Brakes India Ltd, private sector enterprises of the

TVS group are located at Aviyur and Kanjanaiyakampatti in Kariapatti taluk. The former manufactures high density bolts and nuts while the latter manufactures automobile brakes. There are 19335 registered small scale industrial units as on 31 December 1999 engaged in the manufacture of a very wide range of products. Cottage and village industries are dispersed throughout the rural areas. Some common cottage industries are: making of boxes and other articles from Palmyra leaves, metal artifacts fashioned from copper and brass, and aluminium vessel manufacture for domestic use. Gold jewelry making enterprises are concentrated in Virudhunagar, Rajapalayam, Srivilliputtur and Aruppukottai. The Traditional lock making enterprises are situated in Rajapalayam town. Virudhunagar, Rajapalayam, Sattur, Watrap, Aruppukottai and Kamudi are important centres for wholesale and retail trade. Cotton, groundnut, chillies and spices are the main agricultural goods of trade. Matches, crackers, cement and textiles are marketed both within and outside the State. Two warehouses at Virudhunagar and Rajapalayam offer facilities for storage of food grains, spices, pulses, chillies, jaggery and cotton.

An analysis of the growth of small scale sector reveals that the significant change in structure and pattern of the industrial development have taken place within the small scale sector in the district. Promising changes in structure and pattern of industries have made a noticeable impact on the production front.

1.1 Strength

- a) Widened highway from Chennai to Kaniyakumari.
- b) Widened road from Madurai to Tuticorin
- c) Completion of Sethu Project.
- d) Extended Port in Tuticorin
- e) Nearest Airport at Madurai – 45 Km.
- f) Availability of skilled labours.
- g) Formation of SIPCOT & SEZ

h) Dispersal of different types of Micro, small and medium clusters in different location of the district

i) 5 TNEB substations are yet to commence

1) Pulvaikarai

2) Sulakkarai

3) Nenmeni

4) Sukaravarpatti

5) Nallamanaickenpatti.

j) SH 42 were converted into NH. 2000 Crores were sanctioned for the extension of two way road into four ways.

1.2 Weakness

a) Non – availability of Technical person

b) Lack in Technical adoption

c) Competition from abroad like china etc.

d) Low infrastructure

e) Low rail connectivity between different states of India

1.3 Opportunity

a) Availability of natural resources

b) Diverged business operation

c) Availability of Manpower

d) Developed IT field

e) Better export chance

f) Availability of waste land

g) Near to Tuticorin Port

h) Strong Presence of Enterprising People

i) Extension of Srivilliputhur to Parthibanoor road as four ways

1.4 Threat

a) Tough competition

b) Non – availability of credit

c) Non presence of big industrial estate

The district is not witnessing the strong presence of Medium scale enterprises. There are 9 large scale enterprises in this district. They are mostly engaged in manufacturing Auto component, cotton and textile products, cement, and surgical cotton.

1.5 Major Industrial Groups in Virudhunagar District

1. TVS Groups
2. RAMCO Groups
3. Jeyavilas Groups
4. Naatchiyar Groups
5. Arumuga Group of Industries
6. Subburaj Cotton Mills Group
7. Standard Group of Industries
8. Arasan Group of Industries
9. Cement factory

1.6 Service Enterprises

Virudhunagar district is witnessing a strong presence of service enterprises and foot loose industries. Major contribution has emerged from service enterprises. The following service enterprises are having visible presence in Virudhunagar regions: Hotel, Hospitality enterprises, Hospital, restaurant, Industrial consultancy,

educational instructions ,web site developing, two - 4 wheelers servicing and repairing, tutorial, BPO, private telephone, Marriage Bureaus, electric and electronic goods servicing and repairing, Travel Agency, Gas Agency, Construction consultancy, Marriage items hiring, industrial Testing Labs, Advertising Agencies, Marketing Consultancy, Typing Centers. Desk Top Publishing, internet Browsing/Setting up of Cyber Café Auto Repairs, Services, Garages, Laundry & Dry, X-Ray clinic, Cleaning, Animal dispensary, Weigh Bridge, Blue Printing and enlargement of drawing/designs facilities, Operation of Cable TV Network, Beauty Parlours and Crèches.

1.7 Potential areas for service industry

BOP, Hotel, Hospitality enterprises, Hospital, IT enabled, Documentary Films on themes like Family Planning, Social Forestry, Energy Conservation, and Commercial Advertising, industrial Laundry , Tailoring., Pathological lab, integrated diagnostic centre, Sub-contracting Exchanges (SCXs) established by Industry Associations, Beauty Parlors and Crèches, fitness centre for men and women, Glass engraving, Ladies and gents Hostel , House Keeping and Office and equipment maintenance , Interior decoration, Industrial design and layout making, Logistic centre, Material Handling, Metal coating, Office Automation, Parcel servicing and private carrier, upholstery , Power System maintenance, Manpower agency, Weighing bridge repairing and maintenance, digital printing, Embroidering and chamki work , repacking of agriculture produce, Glass engraving, multipurpose diagnostic centre.

1.8 Suggestion for Industrial associations from MSME

1. Creation of Common display centre within SIDCO industrial Estate, Industrial Association and DIC.
2. Fund support for undertaking adhoc studies.
3. Skill up gradation – participatory model Industry-Institution – MSME –DI - E & T programs may be allowed to conduct by Industrial association and MSE by themselves.
4. Project specific allocation for introducing hybrid business development for Tribal, Rural and artisan clusters.
5. Scheme for community enterprises in respect of privileged groups and Tribal community.
6. Fund support for establishing Community enterprises at Tribal regions.
7. More support from NSIC, Re introduction of hire / purchasing scheme.
8. PMEGP scheme may be revised and KVIC may be allowed to fund only rural enterprises and State May be permitted to implement the scheme for promoting more MSEs at regional Level.
9. Creating common software for tracing the industrial sickness.
10. Conducting Integrated modular rural development programs.
11. Establishing Business Incubation within the premises of Industrial Estates.
12. Preparation of need based project proposals for establishing Medium scale enterprises.
13. Creation of multiple linkages with educational institutions, R &D centers.
14. Developing forward linkages with user groups.

2. SPECIFICATIONS OF THE MOTOR

The particle size Current – 4.2 A
Voltage – 230 V
Capacity - 1.5 Hp
Speed – 1500 rpm

3. DESIGN OF PV PANEL

The design of solar panel involves the following steps:

1. Load calculation
2. Inverter design
3. Calculation of battery ratings
4. Charge controller efficiency
5. Design of PV panels



Figure 1 Design of solar panel

Consider the motor load having 1.5 Hp.

1 Hp = 746 Watts.

1.5 Hp = 1.5 x 746 Watts = 1119 Watts.

Total Watts of the motor = 1119 Watts.

Total Watts hour of the motor load = 8952 Wh

Consider the motor operates for 8 hours

Inverter rating = $1119/0.8=1397.78$ VA

Power factor = 0.8

Consider inverter efficiency of 93 %

Output of the battery = $8952/0.93=9625.81$ Wh

Consider a battery rating of 12 V, 100Ah

System voltage = 24V

20 Batteries are connected in series to obtain 230V

Depth of discharge of battery = 75 %

Rated Ampere hour of battery considering Depth of discharge
= $0.75 \times 100 = 75$ Ah

Actual Ampere hour of the battery = $9625.81/230=41.85$ Ah

Number of battery = $41.85/75=0.6$ (approx-1 battery)

Considering, the autonomy of 5 days for this case. Hence, the number of strings would be $5 + 1 = 6$. Number of strings = 6

Number of PV panel

Controller efficiency = 0.97

Input to the battery = $9625.81/0.8 \times 0.97=12404.39$ Wh

Battery efficiency = 80%

Number of sun shine hours = 5

System voltage = 230 V

Ampere hour of the panel = $12404.39/230=53.93$ Ah

Ampere rating of PV panel = $53.93/5=10.79$ A

Consider a PV panel of voltage 15V, 5A, 75w

Number of panels in parallel = $10.79/5=2.16$ (approx-3)

Number of panels in series = $230/15=15.33=16$

4. CONCLUSION

This paper dealt with the use of nano coated motor in the pyro industries and design of Solar panel for that nano coated motor which were used in the pyro industries located in Sivakasi. South Tamil Nadu was becoming an important solar hub in the world. Solar power generation units were constructed in South TN for continuous and uninterrupted power supply to the country. Recently, some HVDC cable transmission of power project from Sri Lanka to Madurai grid were under in initial state to get power from Sri Lanka to India in future. Set up of nano Lab is rare, new and uncommon. It is also an emerging technology. Fabrication of powder needs extra machines which are not popular among common people. It will become popular in the coming future. Nano coated motors can bring the following changes in the conventional machine tools:

1. Accuracy and quality of output can be improved
2. Improves the life time of the plant
3. Reduces the maintenance cost

The proposed work can be extended in future as follows:

1. Coating of stator winding of induction motor with enamel filled with various nano fillers such as ZrO₂, ZnO, Al₂O₃, SiO₂, SiC and so on.
2. Testing of nano coated motors – load test, blocked rotor test, no load test, temperature withstanding test
3. Measurement of stator resistance
4. Equivalent circuit parameters
5. Speed control of nano coated motor
6. Comparison of both nano coated motor and normal induction motor
7. Harmonic reduction by using nano fillers
8. Measurement of EMI and EMC
9. Estimation of losses in both motors and its comparison
10. Implementation of solar panel for the nano coated motor.

5. ACKNOWLEDGEMENT

We express our sincere thanks to the God, the Almighty, and Lord Jesus Christ. This paper is dedicated to the hard working people of Virudhunagar district. We express our gratitude

towards our Tamil Scientist Dr. A.P.J. Abdul Kalam. We express our deep heart feelings towards His death and the people who have lost their lives in Tamil Nadu floods, 2015.

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Effects of ultrafine limestone powder on some properties of Portland cement

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Abstract: Limestone is usually ground with clinker, gypsum and mineral additives to produce blended Portland cement [2,3,4,7]. In this case, the main size of limestone is 20÷30 µm, limestone plays a role as filler. However, using ultrafine limestone powder (with the main size is about 2÷3 µm) creates many different properties, it becomes a mineral additive to increase the quality of cement. This paper presented some results about the effect of ultrafine limestone powder from Yenbai with a reasonable amount on some properties of Butson portland cement. When we used ultrafine limestone powder with a reasonable amount, the early strength of cement increases 20%; simultaneously, the bleeding of cement decreases.

Keywords: cement, additive, ultrafine limestone, properties, strength

1. INTRODUCTION

Cement production technology has a long life and has much improved compared to the past in order to improve productivity, and the quality of cement. However, two major problems in cement production is always attracted, the reduction of production cost and waste pollution. One of the effective measures to solve this problem is the use of mineral additives [7].

This paper refers to some results about the effect of ultrafine limestone powder on some properties of cement. The goal raised the possibility of using ultrafine limestone partially substitute clinker in cement, contribute to improve some properties of cement, simultaneously, reduce CO₂ emissions from the process of cement production.

2. EXPERIMENTAL

2.1 Materials

Butson portland cement, Vietnam standard sand, Yenbai ultrafine limestone powder.

Tab. 1 shows a chemical composition of Butson portland cement.

Table 1. Chemical composition of Butson portland cement

Chemical composition (%)							
CaO	SiO ₂	Al ₂ O ₃	Fe ₂ O ₃	MgO	K ₂ O+Na ₂ O	SO ₃	LOI
64,88	21,24	5,27	3,19	2,26	0,94	1,88	0,33

Tab. 2 shows particle sizes and chemical compositions of Yenbai ultrafine limestone powder.

Table 2. Particle size and chemical composition of Yenbai ultrafine limestone powder

Particle size (%/µm)					
%<	10	25	50	75	90
µm	0,545	0,773	1,871	3,040	4,834
Chemical composition (%)					
LOI	SiO ₂	Fe ₂ O ₃	Al ₂ O ₃	CaO	MgO
43,53	0,18	0,009	0,039	54,98	0,5

2.2 Methods

Some physical properties: TCVN.

Structural characteristics, composition phase/mineral: SEM, DTA, XRD.

To determine the particle sizes of 0,4 ÷ 2000 µm: equipment use 750 nm wavelength laser source by light scattering principle.

3. RESULTS AND DISCUSSION

3.1 Effect of ultrafine limestone powder on some properties of cement (consistent, setting time, spread and bleeding, strength)

The influence of addition of ultrafine limestone powder (UL) to the Portland cement was determined through the examination of consistent, setting time, spread and bleeding, strength is shown in Tab. 3.

Table 3. Effect of ultrafine limestone powder (UL) on some properties of cement

Sample	UL (% mass)	Water demand (% mass)	Setting time (min)		Water/Cement	Spread (mm)	Water/Rigid	Bleeding (%)
			Initial	Final				
S0	0	27,20	96	150	0,5	86,25	0,9	16,01
S5	5	26,00	55	115	0,5	79,00	0,9	12,72

S10	10	26,40	52	110	0,5	63,75	0,9	5,68
S15	15	26,80	45	94	0,5	53,50	0,9	3,22
S20	20	26,80	40	104	0,5	59,38	0,9	2,03
S25	25	28,00	35	98	0,5	58,13	0,9	1,16
S30	30	29,20	44	90	0,5	46,63	0,9	1,17
S35	35	29,60	37	93	0,5	51,38	0,9	0,56

3.1.1 Normal consistency

The water requirement, determined on the fresh paste, is reported in Tab. 3. It seems that ultrafine limestone powder reduces water requirement compared to Portland cement. Moreover, increasing the amount of limestone requires much water.

3.1.2 Setting time

From Tab. 3, it indicates the initial and final setting time of cement pastes at different amount of limestone. The obtained values show that both initial and final setting times were decreased with an increase in the amount of limestone. It can be concluded that limestone fills the pores between cement particles due to formation of carboaluminates, which may accelerate the setting of cement pastes.

3.1.3 Spread of cement paste

The results from Tab. 3 show that the spread of cement pastes was decreased. Because of using ultrafine limestone powder, with w/c = constant, caused higher specific surface area, thus the thickness of the water layer on cement particle surface decreases, which

increases the internal friction, leading to reduce spread of cement paste.

3.1.4 Bleeding

When we using ultrafine limestone powder, the bleeding of cement pastes decreases. The more amount of additive, the more reduction of separated water. The amount of separated water greatly reduced in samples of 5; 10; 15% cement replacement additive (the bleeding decreased from 16% to 3,2%); then, it slowly reduced in the other ratios.

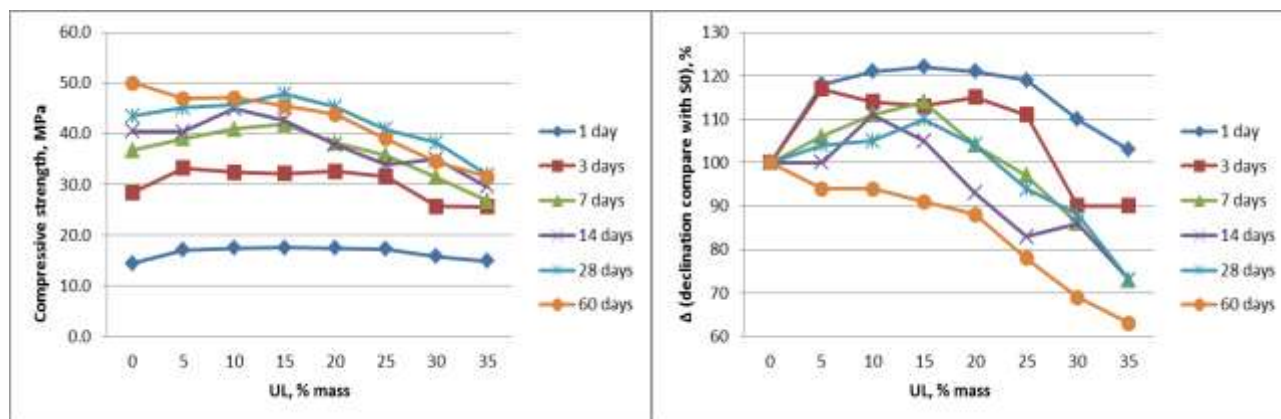
This result is caused of the ultrafine limestone particles increases the surface area, the amount of adsorbed water around the surface of the particles also increases. In contract, the formation of monocarboaluminate ($C_3A \cdot CaCO_3 \cdot 11H_2O$), hemicarboaluminate ($C_3A \cdot 0,5CaCO_3 \cdot 0,5Ca(OH)_2 \cdot 11,5H_2O$), which increases the water holding capacity of cement paste, so the amount of separated water decreases.

3.1.5 Strength

The influence of the ultrafine limestone powder addition on the compressive strength of cement is shown in Tab. 4 and Fig. 1.

Table 4. Effect of ultrafine limestone powder (UL) on compressive strength of cement

Sample	UL, % mass	Compressive strength, MPa						Δ (declination compare with S0), %					
		1 day	3 days	7 days	14 days	28 days	60 days	1 day	3 days	7 days	14 days	28 days	60 days
S0	0	14,4	28,4	36,7	40,5	43,5	50,0	100	100	100	100	100	100
S5	5	17,0	33,2	39,0	40,4	45,1	46,9	118	117	106	100	104	94
S10	10	17,4	32,4	40,9	44,9	45,6	47,1	121	114	111	111	105	94
S15	15	17,5	32,1	41,8	42,6	47,8	45,5	122	113	114	105	110	91
S20	20	17,4	32,6	38,2	37,8	45,3	43,8	121	115	104	93	104	88
S25	25	17,2	31,6	35,7	33,8	40,8	39,0	119	111	97	83	94	78
S30	30	15,8	25,7	31,4	34,9	38,2	34,5	110	90	86	86	88	69
S35	35	14,9	25,6	26,8	29,6	31,8	31,5	103	90	73	73	73	63



(a) Compressive strength

(b) Declination

Figure 1. Effect of UL on compressive strength of cement

Tab. 4 and Fig. 1 show that:

Ultrafine limestone powder increases compressive strength at early ages (1; 3 days). Lower declination are obtained with higher addition levels.

Ultrafine limestone decreases compressive strength of cement at the later age (60 days). Higher amount of addition, lower declination.

When we use addition with amount lower 15%, the compressive strength of cement increases at early ages, decreases at later age.

This result is caused of some reasons:

Limestone improves the hydration rate of minerals C_3S , C_3A , C_4AF [7].

The presence of ultrafine limestone was slowed down the formation of C_3AH_6 ; simultaneously, the formation of monocarboaluminate ($C_3A \cdot CaCO_3 \cdot 11H_2O$), hemicarboaluminate ($C_3A \cdot 0,5CaCO_3 \cdot 0,5Ca(OH)_2 \cdot 11,5H_2O$) [1,3,4,6].

The effect of aggregate and crystalline nuclei of limestone powder is a favorable condition for the formation and development of crystalline hydrate. It gradually fills the pores between particles of cement, creates the dense structure. Moreover, with the ultrafine size, this band of limestone might contribute to improve the grain composition, arrange tightly structure and reduce the size of the pores in cement hydrated.

Increasing levels of additives cause the dilution of minerals, which reduces the intensity of cement hydrated when excessive levels of additives.

The decline in the intensity at the age of 60 days likely due to the conversion of the mineral form of ettringite to calcium monosulfoaluminate, calcium monocarboaluminate accompanying volume change ($d_{ett} = 1,77 \text{ g/cm}^3 < d_{mono} = 2,17 \text{ g/cm}^3$), also due to slowing C_3AH_6 formation, or the transformation of calcium monocarboaluminate from thin sheets to form shape metal rod will cause residual stress [6]. These changes cause the volume reduction and create pores in cement hydrated. Since then, the strength of cement hydrated tend to decrease when combined with limestone. This is usually seen in the report on the recent studies.

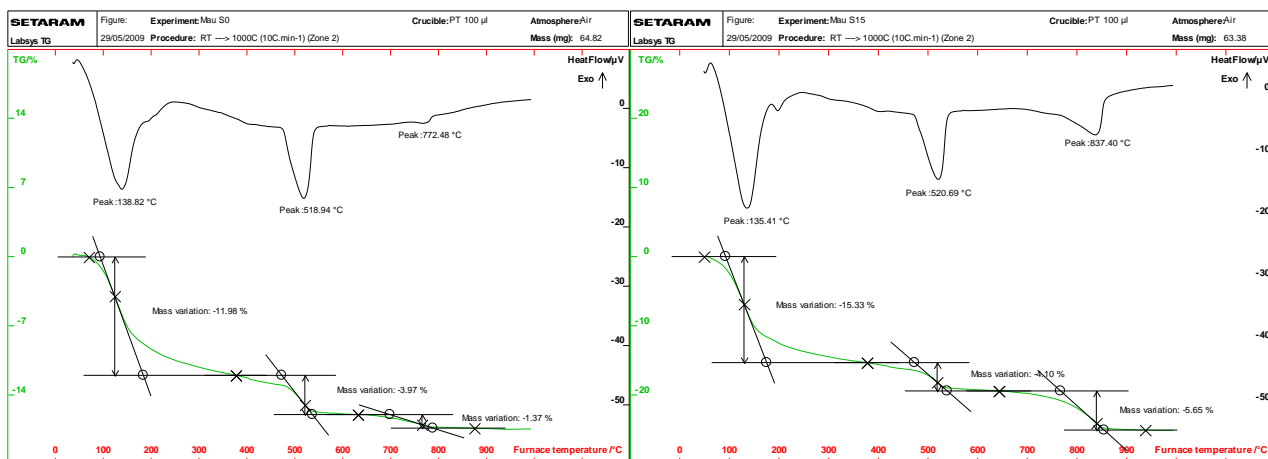
3.2 The effect of ultrafine limestone on the process of the hydration and the formation of crystals

3.2.1 Differential thermal analysis (DTA)

At a temperature of less than 250°C , the amount of loss H_2O is free water, bound water of calcium silicate hydrate CSH (B), calcium aluminate hydrate (ferrite) [5].

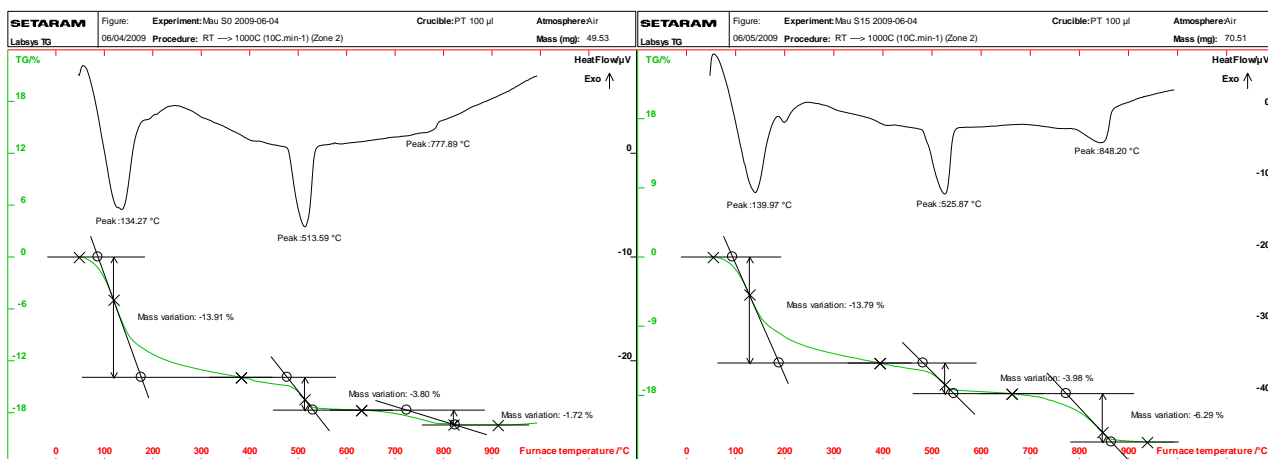
From 250°C to 500°C , the amount of water loss is mainly caused by the decomposition of $Ca(OH)_2$, and a part of the remaining calcium silicate hydrate minerals [5].

From 500°C to 1000°C , the amount of LOI is caused by the hydration of the remaining compounds and CO_2 . CO_2 is considered to be the result of the decomposition of $CaCO_3$ in the cement hydrated; created by the reaction between $Ca(OH)_2$ and CO_2 in air and $CaCO_3$ in additives [5].



(a) DTA of S0 at 7 days

(b) DTA of S15 at 7 days



(c) DTA of S0 at 14 days

(d) DTA of S15 at 14 days

Figure 2. DTA of the samples at different ages

It is considered that LOI of cement is the loss of free water at temperatures below 100°C, and dehydration at below 500°C in the compounds of calcium silicate hydrate CSH (B), calcium aluminoferrite (ferrite) and

Ca(OH)₂. Hence the minus can be seen as separate chemical water.

LOI of cement samples, after the ages of hydration, at the temperature below 500°C follows in table 5:

Table 5. LOI of S0 and S15

Day	LOI, %					
	S0			S15		
	<100°C	500°C	100 ÷ 500°C	<100°C	500°C	100 ÷ 500°C
7	1,2	14	12,8	2,3	17	14,7
14	2,5	15,4	12,9	1,3	15,1	13,8

It is clear that, when temperatures range from 100°C to 500°C after 7 and 14 days, the amount of losing water of S0 sample (pure cement) is less than S15 sample (cement has 15% limestone).

the content Portland cement minerals in the samples which have the additive is smaller than test samples. The figure indicates that the additive has stimulated the process of hydration and solid, accelerated these processes.

From DTA diagrams in Fig. 2, the weight loss in temperature ranges below 500°C of samples which have the additive is higher than pure cement samples, while

3.2.2 XRD analysis

The results of XRD analysis are shown in Fig. 3 and Fig. 4 below:

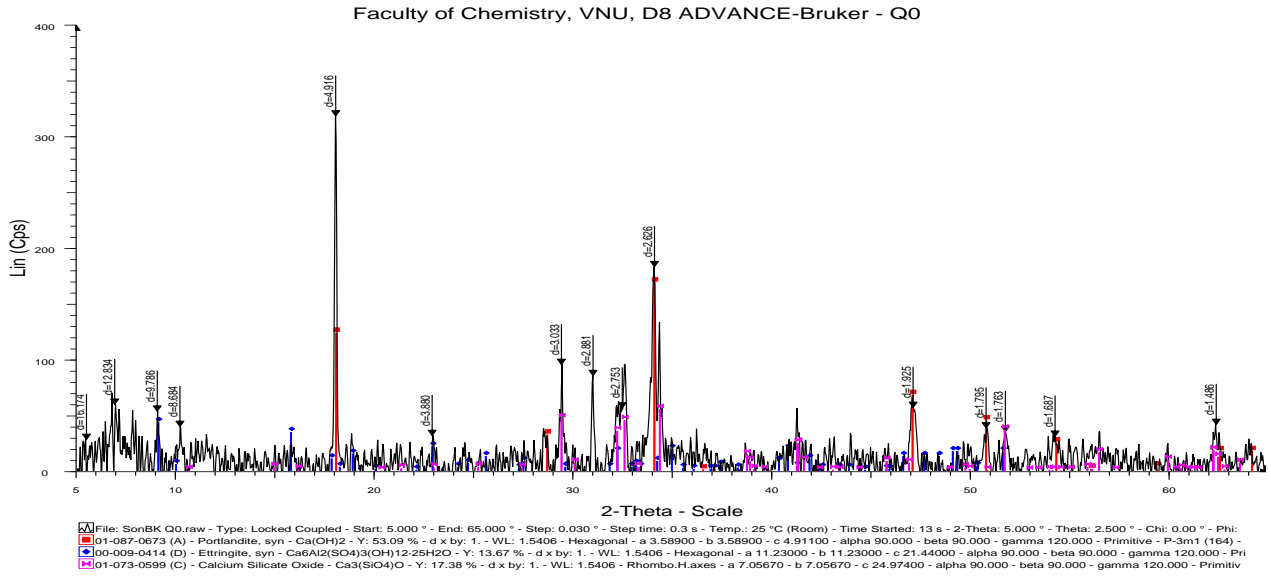


Figure 3. XRD of S0 at the age of 7 days

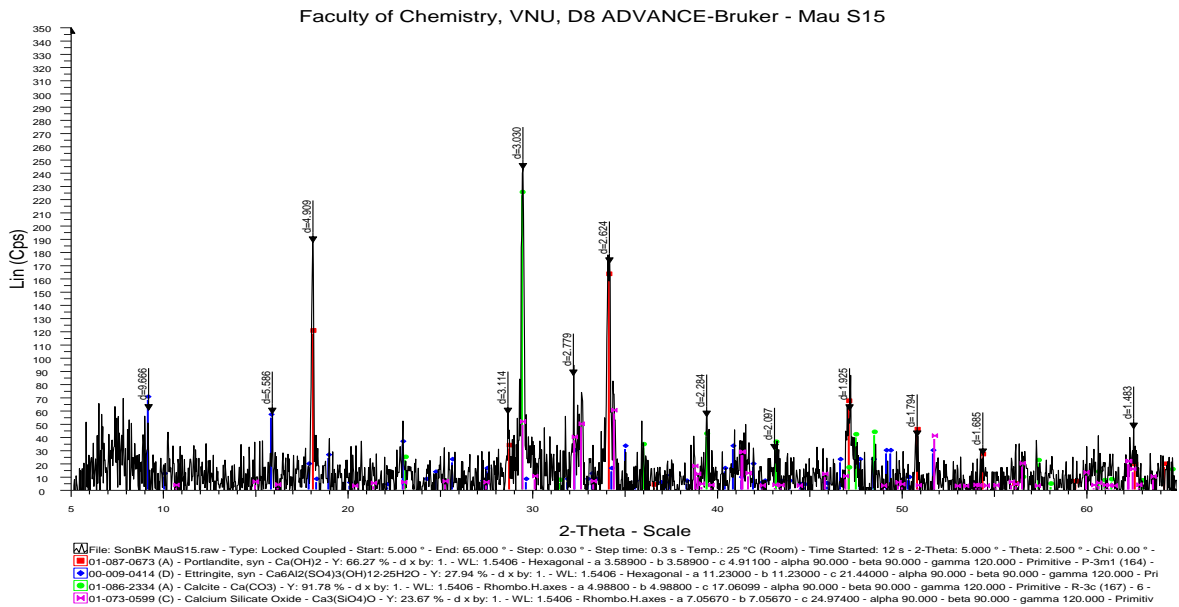


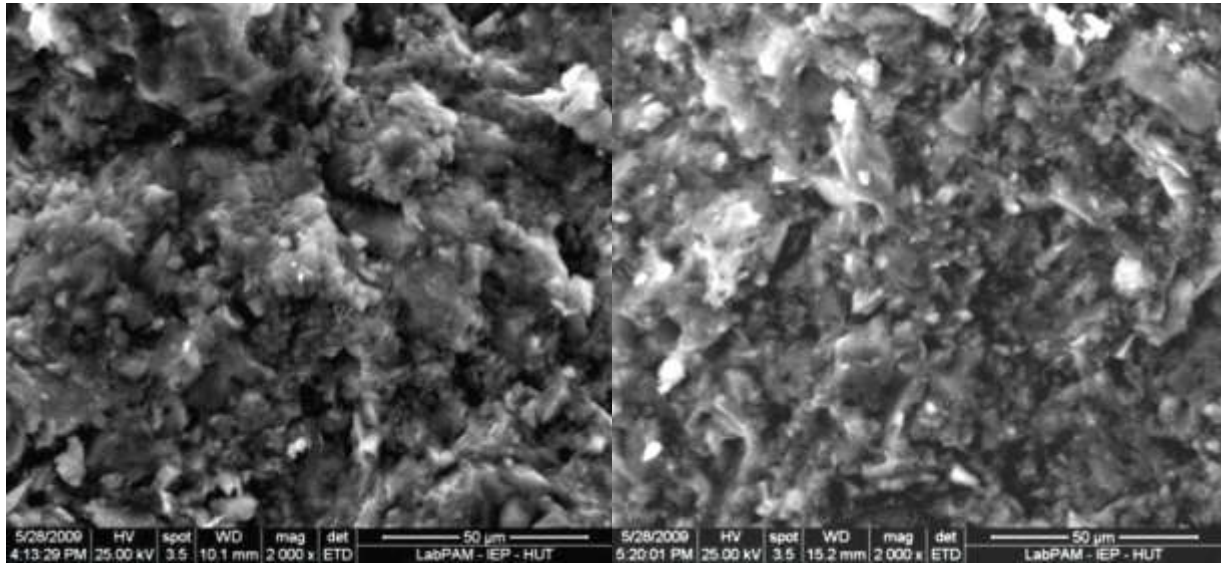
Figure 4. XRD of S15 at the age of 7 days

The content of Portlandite crystals Ca(OH)₂ are found in the pure cement sample is higher than S15 sample, it is a possibility that a part Ca(OH)₂ combined with CaCO₃ form hemicarboaluminate (C₃A.0,5CaCO₃.0,5Ca(OH)₂.11,5H₂O) [4,5,6]. It is

consistent with previous studies and test results about strength.

3.2.3 SEM results

The results of SEM are shown in Fig. 5.



(a) S0

(b) S15

Figure 5. SEM pictures of the 7-age samples

After 7 days in hydration, the structure of S15 cement sample is closer and pore density is less than the structure of S0 cement sample. It would appear that limestone plays a role in initial nucleus actively and more evenly; moreover, it contributes to fill the pores.

4. CONCLUSION

Used up to 15% additives still maintains the basic properties of cement followed by Vietnamese standards.

Improved approximately 10÷20% strength at the early ages when we used to 15% additives.

The dehydration reduced. Specially, the bleeding rate reduced significantly from 16% in the pure cement sample to just under 3% when we used to 15% additives.

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Critiquing Recalling as Mechanism in Answering Questions during Evaluation

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Abstract: Evaluation has been the key measuring instrument employed to determine knowledge, skill, and competence levels in Ghanaian schools. By design, conventional assessment has been structured for students to recall studied materials and re-produce it through oral presentation, inscription, and/or demonstration. This is also the orthodox order by which appraisal has been undertaken to declare pass and qualification. The mechanism by which performance, knowledge, skill, and competence are determined based on volume of information to recall appears to be a limiting factor in measuring knowledge, skill, and competence especially in Technical and Vocational Education Training (TVET). Relatively, it is a common feature in world of work where labour has the leverage to refer from documented materials and other authorities and experts to deliver as expected. The study thus, is an inquiry attempting to look into the means of measuring performance, knowledge, skill, competence, and standards without depending much on absolute recall. It is a direct attempt to reduce rote learning drastically and prepare students for life other than examination. Being literally qualitative and quasi-experimental research, the inquest will adopt observation, descriptive, interpretative, and partial experimental research.

Keywords: Evaluation, Student, Teacher, Recall, and Learning.

1. INTRODUCTION

Many an authority of education will describe education as a means by which people who enroll (students) into school could be trained and guided to acquire knowledge, skill, and competence (Smith, 2015, Roni, 2011, & Tesha, 2016). By design, education also imbues and sharpens the capacity into being adaptive and poised physically, mentally, emotionally, fit, and responsible (Smith, 2015, Roni, 2011, & Tesha, 2016). To declare the student who must have gone through the system passed well enough to exit the confines of the school, the former ought to have proved that all learning outcomes espoused must have been acquired reasonably and evaluation is the key yardstick for undertaking search measurement. Since the inception of formal education, summative assessment has been the key tool by which performance and capacity is determined. Recently, a mix of formative and summative assessments in the ratio 4:6 have been instituted in many institutions in Ghana and that is what Takoradi Polytechnic also adopts. The structure by which these assessments are executed for appraisal have many questions among them is the challenge of volume of information that can be memorized and its relationship with pass, adaptation, and performance which have been encapsulated by Novak, (2011) p. 1., as think,

feel, and act. At present, dominance of the concept of thinking (recall) and act (delivery) with limited reference to feel (how or methodology) form the fundamental challenge of illiterate graduate and the reason why employers look for five (5) to ten (10) year working experience.

By and large, qualification has been linked directly to the ability of the student to recall as much as possible and present as directed by the marking scheme in making required grade for transition to the next level. Instinctively, this has introduced varying dynamics into schooling and evaluation and subsequently knowledge, skill, and competence. Passing adequately has been the goal and thus, the conventional practice is to grasp as much as possible, recall, and deliver orally and/or inscriptively. Often, students eagerly ask for notes or pamphlets, study the contents, and deliver on demand. Summarily rote learning has become so entrenched and prevalent defeating grossly the key aims and objectives of education. According to (Mayer, 2002), retention focuses on the past and transfer focuses on the future. Within the context, retention looks at memorizing and transfer requires memorization to deliver in performance. Now, the end is prioritized over the means and as such, many students have been drawn into the penchant of cheating: influencing facilitators and examination

officials to buy questions and marking schemes, manipulate results, and refer to foreign materials and discussions while examination is in session. Ultimately, ill-equipped graduates and professionals get churned out; hence, the emerging phenomenon where industry requires five (5) to ten (10) year working experience before hiring. Industrial players for some time have bemoaned passionately that graduates do not measure up to standards required for the world of work. Correlating with the context is the opine caveat by Novak (2011) p.1., that expresses learners, teachers, subject matter selected, social milieu, and evaluation to be benchmarks of education theory. Indeed, every graduate should have certificate serving as evidence in support of satisfying the benchmarks Novak has advocated. However, direct relationship between evidential certificate and evidential result from productivity is core of the controversy. The sensitive and unfortunate situation is particularly dire in TVET education like the polytechnic where knowledge, skill, and competence are the targets.

Increasing dangers from over-emphasizing skill and competence performance appears to have its associated limitations likewise. To illustrate its effect, Battino, (1992) p. 1., argues that understanding and recalling elements of the periodic table in chemistry is very essential in appreciating technical and technological processes and theories of chemistry. Factually, practical undertakings may be helpful but to assimilate and memorize cannot be ostensibly missing in this endeavour. That is why the contention of meaningful learning by Mayor, (2002) p.1., where convergence is made between the Taxonomy of retention and transfer appears to be on spot. If meaningful is relegated to the background, then brace yourself for any of the three possibilities: no learning, rote learning, and meaningful learning (Mayor, 2002, pp. 1-2).

The struggle in Ghana points to the trajectory where the focus is on pass to make it to the next level (academic progression and/or world of work). Under the regime of president John Agyekum Kufour, it was believed that making high school duration seven (7) years that is from age 12 to 19 should equip students comprehensively for progression into tertiary notably university. As at now, the then government, Ministry of Education, and Ghana Education Service are yet to produce any scientific evidence to support the claim that increment in volumes that passed West Africa Senior Secondary Certificate Examination (WASSCE) as a result of four (4) year senior high school education had meaningful learning. The damage is revealed in placing emphasis on rote learning to the detriment of meaningful (smart) learning ultimately leading to no learning. A reflection seen when industry provide feedback on performance on students on industrial attachment and internship. We are often told by industry how frequently students from the regular universities use grammar to express and explain issues but struggle to deliver on the job whereas the HND students deliver on the job and also struggle to express themselves freely.

2. RESEARCH DESIGN

As a typical applied research, the broadly qualitative study has somewhat worked along quasi-quantitative approach utilizing experimental, observation, descriptive, and interpretative design and method. It has elicited factors that fan recall and rote learning leading to the chaos being experienced and suggest remedies. It is hoped the outcomes will give stronger basis and support for CBT and formative assessment as the paradigm in TVET especially at the Polytechnic.

Employment of qualitative and quasi quantitative approaches are revealed in sessions as facilitators (teachers) and learners get interacted. During sessions, a common experience is to get students ask lecturer to convert the materials into notes even though full references have been provided in support of study material. Students will be sincere to confess regardless of provided references; we did not really consult the reference for information and knowledge expansion. On the contrary, they prefer to get busy during revision and examination period to recall as much as possible. Approach to evaluation particularly: quizzes and examinations has been much disturbing as though the world of the student must have ended. People strive to burn the mid-night oil, try to cheat, and worst of all, unable to apply whatever material they must treated creditably during the quiz or examination in future even with reference materials in support. Most of all, many lecturers do not see the need to limit the application of summative assessment to the advantage of formative assessment: a pattern that became obvious during curricular review in transition from polytechnic to technical university in 2016. And the relevance is seen because many of the lecturers have the same background as the students and would wish to work with convenience. During the end of year examinations which ended in June, 2016, out of eight papers (8) a lecturer invigilated, it was one that seems to have professionally well composed question for the examination. A related very disturbing phenomenon is examination result manipulation by lecturers and in some instances, examination officers. Generally depending on summative assessment puts lecturer in charge and gets students forced to explore but without evidence to support legitimacy of the so called acquired knowledge.

3. RESULTS AND DISCUSSION

As part of the inquest for this paper, a quiz was conducted for mid-semester examination and presented for your perusal.

TAKORADI POLYTECHNIC

MID-SEMESTER EXAMINATION QUESTION

SCHOOL: Applied Arts	YEAR: HND 1
DEPARTMENT: Fashion Design and Textile Studies	
Semester: Two (2)	

PROGRAM: Fashion Design and Textile Studies	
Section: 2015/16	
COURSE:	Drawing and Illustration
Course Code: FDT 106	
Duration: 1½ Hours	Credit Hours: 3
NAME OF LECTURERS: Kenneth Bright Boateng and Ahmed Jibril	

INSTRUCTIONS

You are permitted to come in with all your reference materials with the exception of computers and smart phones. Also come along with relevant drawing and painting materials and instruments. Answer all questions

1. State and explain the main relevance why in illustrations, the legs are portrayed to look taller than the torso/trunk in fashion.
5 Marks
2. List five (5) elements of design and show how to demonstrate each visibly in garments and accessories with two (2) points each.
10 Marks
3. Identify with two (2) points each how colour illusion can be used for the following:
 - a) Increase girth of an extreme slim silhouette
 - b) Reduce height of a very tall person
 10 Marks
4. State two (2) ways by which you can adopt balance to reduce a protruding waist of a lady conveniently.
5 Marks
5. State and explain with two (2) points on how to apply occasion and function in bridal apparel. Support your answer with credible examples.
10 Marks

The findings from the examination have been treated as follows:

Pedagogy and andagogy are key training doctrines which aid directing learning form known to the unknown; simple to complex; concrete to abstract. Virtual skill required to express little or much vividly for the understanding of students is a teaching artistry that requires observation, experience, and versatility. Knowledge and use of these principles does depend on age but capacity of the learner and hence, the difficulty in its application during training of disengaged students as pertain in the polytechnic. Looking at average age students in the polytechnic makes it easier to conclude that they are matured which is highly subjective. Understandably, dependent on formative assessment brings knowledge, skill, competence, and adaptive cleverness (versatility) but the former is inadequate that is why the significance of summative assessment cannot be over-emphasized. Granting documented materials to facilitate

revision and personal studies are not evil but needs to be highly skewed to reflect capacity and strength of student to stimulate personal drive for quality knowledge, skill, and competence. Of the nine (9) students whose project report were vetted in 2015/2016 academic year, only one had good command over oral and written English. Seven (7) were not impressive but two (2) could not write a complete sentence with grammatical flaws even though they have adequately delivered the final collection (end of programme project work).

Absenteeism and truancy is a regular feature in training institutions across education with teachers and educational authorities employing varying tools for its control. To root out this debilitating quagmire, trainers and institutions may want to consider alternative motivation where no documented material in the form of notes, pamphlets, leaflets, and handouts are issued to students but the latter is required to deliver answers to smart quiz within 30min at the beginning of first session of every month. From observation, many smart students of very large class size stay out of attention and sneak in and out of class at will but make the required grades all the time. Varying the rules of engagement to demand performance through direct contact as seen in formative assessment should literally reduce this menace of education.

In the past, a regular practice in evaluation is to offer mark up for brilliant performance but it was discovered that this simply became another avenue for teachers to hand over marks freely to their favorites spanning from the well-dressed, athletes, disciplined, child with special needs, errand runners, and even concubines. A more scaring phenomenon is where teachers load questions requiring voluminous written statements that the former would not have the time to mark and award appropriate marks. In short, the teacher just awards marks based on familiarity and fraternity other than performance. The compelling evidence is so staggering knowing that some failures and excellence do not necessarily merit the award with its subsequent tag.

Note taking, pamphlets, leaflets, and handouts have additionally problems creating tremendous challenges to education authorities and the more allowed to thrive, the worse. The problems become apparent just at the beginning of the semester where it takes three (3) weeks or more for average regular student to report fully for lectures even though only the first week is required for registration. They walk casually into class late and then sit oblivious of their environment chatting, fondling their smart phones, and/or absent minded. 'Anyway, I will get the notes from a friend to prepare for the examinations' – that is feedback when questioned. Albeit offensive, reading into it should reveal a structural problem arising from teachers and institutional authorities. If it is permissible for students to be compelled to buy handouts, leaflets, and pamphlets with some attaching award of points and marks to it, you could not be asking for a lesser trouble. This practice reduces discipline and makes

the vulnerable susceptible to abuse by fellow students and in some cases, teachers and education authorities.

The importance of rote learning is being stretched beyond reason and many a teacher has not seen it to be a time bomb. As illustrated by local parlance in Ghana: 'chew, pass, and forget'; many a student goes through great length to grasp and assimilate as much as possible. Trying to capture and memorize contents is not adequate to guarantee productivity is a challenge because that has been their experience from the basic levels. At the polytechnic where beyond completion of programme is on the job performance requires additional skill and competence that can and must convert raw or semi-finish to finish. Well, some teachers contend that well designed questions from open ended to close ended within the context of knowledge, skill, and competence demonstrated by the learning outcome should draw appropriate responses from the answers students provide. But, a counter contention is the student has recalled and provided the answers as being demanded but cannot perform the task in the world of work.

Since 1993 when I began practicing professional teaching from basic through secondary to tertiary, am yet to experience examination (spanning from invigilation to awards) where cheating (copying from neighbours and friends; foreign materials; discussion; spying; omission and/or manipulation of results, by students and/or personnel) never occurred. Spying appears to be the commonest where students attempt to steal glances at the work of neighbours. No mean lesser, another regular occurrence is the penchant to talk and talking while examination is in session. Albeit it seldom happens, some students have the boldness to grab others works (exchange) and copy oblivious of the presence of invigilator. But the worst and bizarre are smuggling of foreign materials into the examination and then manipulation of and/or by personnel and results. Even at the highest (tertiary) level, I have seen students copy on all sort of materials from papers, underwear, skin to sanitary towels and more all in attempt to recall as much as possible without working for it. Some leave the material in quite close proximity to the examination centre (e.g. toilet) and briefly visit to spy. The most disturbing ones are trading of questions, marking schemes, and results by teachers and/or students alike with sex, money, and opportunities not to talk about lazy teachers who manufacture marks and distribute by acquaintance without necessarily reading scripts. The bottom line is the immaculate drive to manipulate the system to secure advantage without working for it. Sanctions for found cases can be very severe ranging from failure of the paper through rustication to outright dismissal but the prognosis appear frankly bleak: the phenomenon does not appear to be halting as in every examination I helped to conduct during my tenures as examination coordinator and chief invigilator, these infractions occurred across all programmes run by the polytechnic.

Anxiety and violence have also crept into the stream of examination. Visibly stressed students who appear broadly worried and exhausted begin to pester teachers and examiners. "What are the questions about? Any possible areas to emphasize in our learning"? In the extreme students get to the wit end and act carelessly. Some try to trade anything for questions, marking schemes, and better results. Others get abused by teachers, examination staff, and fellow students and in the process, people get breakdown. In University of Education in Ghana where mostly advanced age learners enroll most of whom are teachers, students get rushed to hospital during revision and examination period often on worsening heart conditions. In the polytechnic where youthfulness is prevalent, depression is very common. Also common is violence where students attempt to attack fellow students who do not compromise examination sanity. Vigilant and strict invigilators are seen mean and are sometimes attacked verbally. In an incident I witness, a semester six (6) student caught copying from foreign material in his last paper for the examinations which also to complete his HND education decided to wrestle the foreign materials from the two invigilators who accosted him and the seen was very pitiful.

4. CONCLUSION

- i. Adaptive cleverness by which circumstances could contextualized for sustained optimal performance is extremely essential.
- ii. Relevance of knowledge retention from training is revealed in transfer: application of knowledge in adaptation to evolving trends.
- iii. Session plan, facilitation, and assessment may require review for adaptation to the trends of the times.
- iv. Practical oriented questions with the right for reference from study materials during examination may be helpful after all. In surgical cases, surgeons do not absolutely rely on recall to conduct operations. They sometimes refer to notes and discuss for alternative opinions and/or affirmation.
- v. Timely feedback associated with appropriate counseling to those perceived to have challenges during sessions and assessment as the semester wears on could engender better preparation and confidence during examination.

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Relationship between Information System Components, Trust, and User Satisfaction in terms of Using Green Processes and Technology

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Abstract: Nowadays there are great concerns about environmental pollution which bring attentions on the use of green products and processes. Many researches have been conducted and are being conducted in various industries with different scopes in this term. However, the crucial point is whether green technology and processes are able to adapt in various industries. This research with using quantitative approach attempts to highlights effective variables on trust in green technology and processes, and also impact of trust on user satisfaction at one of the Malaysian university. Thus, considering to Information system success model (IS success model) and previous researches that have been conducted by scholars, this research have chosen Green information quality and Green system quality which are able to influence trust. According to the results obtained from collecting of 150 data from university staff including academic and official staff via distribution of questionnaire, showed that Green system quality, and Green information quality have significant and positive relation on trust. In addition, the impact of Green system quality and Green information quality on trust is significant and positive. On the other hand, the relationship between Trust and User satisfaction is positive and significant; furthermore, trust has a significant and positive impact on user satisfaction.

Keywords: Green environment, System quality, Information quality, Trust, User satisfaction.

1. INTRODUCTION

Nowadays industries consume more energy than necessary, and it causes more pollution. That is why it is important to establish a management system based on green processes and products to reduce the pollutions. Furthermore, the opportunities are provided in green technology. All governments and companies look for ways to reduce waste, because earth's environment today is not in a good state in the term of pollution such as: forest disappearing, water contamination, global warming, and etc that are the major problems for environment. On the other hand, in roofed environment like offices with mechanical ventilation, but without recirculation, devices like computers can cause sensory pollution loads (Al-Ali et al., 2010). In fact, the personal computers (PCs) are found as a strong indoor pollution sources. Besides sensory pollution load of each single PC is 3.4 Olfactus (olf) even when they are serviced for every three months (Bakó-Biró et al., 2004).

Chemical analysis detects there is pollutants emitted by PCs. The most significant chemicals include phenol, toluene, 2-ethylhexanol, formaldehyde, and styrene (Al-Ali et al., 2010). So these types of pollutions have an important negative

impact on the air quality, not only in offices but also in many spaces including homes. Furthermore, (National Public Radio) NPR reports by Chris Arnold in 2004 from Environmental Protection Agency officials say: Computers and computer monitors in the United States are responsible for the unnecessary production of millions of tons of greenhouse gases every year (Ravali et al., 2011).

With the entire world talking about going green, everyone can chip-in his/her bit for the environment and save money and energy. Generally, PCs and other IT equipment consume a lot of electricity and have high carbon emission levels. Accordingly, if there is a potential to enhance the quality of systems used in various industries, there will be a possibility to cut down the emissions. For instance use of Green PCs that are especially designed to minimize power consumption. Moreover, Green PCs draw less power than normal PCs and support sleep modes. A Green PC is a computer that has low power consumption and is environment friendly. It supports sleep modes in which the computer cuts down the power of unnecessary components when it is inactive. Configuring and assembling a Green PC is an easy task.

Many computer components are easy on the environment, save energy and thus, help cut costs. Saving the environment and cutting down on energy consumption has become the need of the hour. With the help of Green PCs, it has now become easier to be environmentally aware without compromising on technological advancements. A Green PC is assembled with environment friendly components. It comes with a number of options such as the option to dim the monitor when it hasn't been in use for some time, the components like CPU, monitor, etc. don't give off high degree of radiation, the components are recyclable, etc. Furthermore, other components like Processors, Motherboards, Monitors, and Hard Drives have come out with new products that consume less power than the earlier manufactured processors and are better or equal in performance.

Besides, if quality of information rises alongside of quality of system, it will be easier to use the systems like PCs. Because in fact information quality is the desirable characteristics of the system outputs. For example: relevance, understandability, accuracy, conciseness, completeness, understandability, currency, timeliness, and usability are all characteristics of a system with high degree of information. On the other hand, capabilities of an information system lead to increase in system usage (Pitt et al., 1995), (Petter, S et al., 2008).

According to the results obtained from past researches by different experts it can be said that user satisfaction can be influenced by some main elements and as a result the performance of individuals remains as a gap related to green behavior. A new framework was developed in this study that connects information quality and the system quality to Trust and also user satisfaction. Another gap refers to consider green product and process for each variable.

2. Literature review

2.1 Information System Success Model

The term IS or information system success is a popular term to measure the information system (Lin et al., 2006). A large number of studies in MIS or management of information system scholarship have developed IS model of success (DeLone et al., 2003; Seddon et al, 1997; Pitt et al. 1995).

Approximately 180 papers about evaluation of IT investment elements have been reviewed that they were published during the 70s and 80s. consistent with the statements of (DeLone et al., 1992) an IS model have been presented with six

variables about IS success including information quality, system quality, system usage, user satisfaction, organizational impact and individual impact.

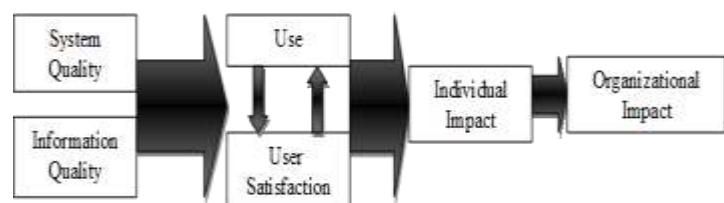
This model joins the comprehensive dependent factors applied by IS experts but on the other hand it also obtained some criticism. First of all, the usage of IS in the model that has been presented by Mclean and DeLone has a lot of interpretations that needs to be examined. It is also mentioned that the IS usage plays a role which is controversial and problematic in the success of modeling system.

In second place, due to the fact that satisfaction of users demonstrates the individual influence of IS in a firm context, therefore it is not essential to investigate on a cause direction from satisfaction of users to individual influence. Finally, the last point that is very necessary is that this model does not describe the relation of individual influence and user satisfaction in a transparent way (Edward et al., 2005). The developed definitions for each of these factors are as follow:

1. System quality: measures of the information processing system itself
2. Information quality: measures of information system output
3. (Information) use: recipient consumption of the output of an information system
4. User satisfaction: recipient response to the use of the output of an information system
5. Individual impact: the effect of information on the behavior of the recipient
6. Organizational impact: the effect of information on organizational Performance (Fig. 2.2).

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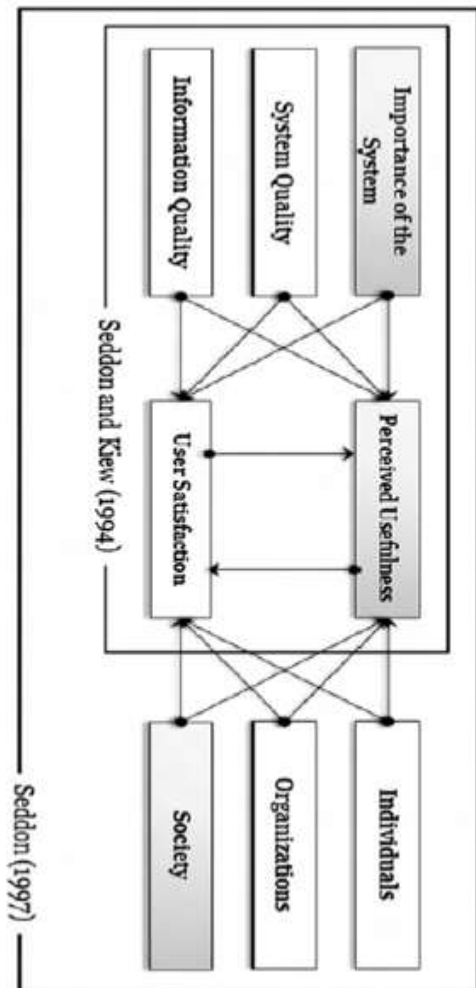
Figure 1: Delon and Mclean IS success model (1992)



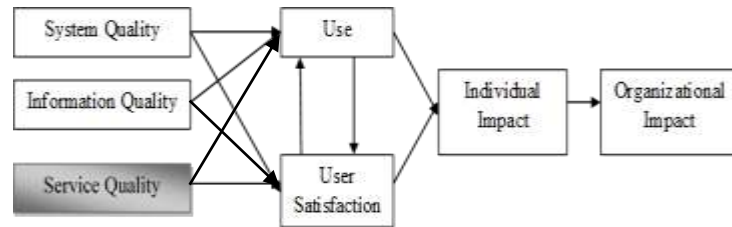
In 1994 Kiew and Seddon tested a modified version of the model which was made by Mclean and DeLone in 1992 that had the three significant differences as follows:

- (a) the usage was replaced by usefulness, (b) a factor crucial for the system was added in order to assist defining the differences in the perception of users related to user satisfaction and usefulness. (c) the casuality that exist among users and user satisfaction was changed by a casuality which was one way. The outcomes that were empirical developed some support for according to model of Mclean and DeLone in 1992. In 1997 Seddon stated a model of IS success in which the influence of society was added as a value of net of the IS (Figure 2.3).

Figure 2: The success model developed by Kiew and Seddon in 1994 and the success model of Seddon in 1997.

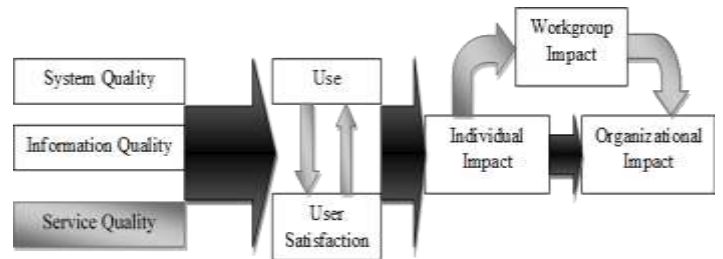


According to the success model of IS by Pitt in 1995 a service quality was added as an element of quality for the model of McLean and DeLone in 1992. For evaluation of service quality the measure tools are shaped from the modified SERVQUAL that were presented by Parasuraman in 1998 and after that the validity was tested (Figure 2.4).



A success model was matured by Myers in 1997 and it was an extension of the McLean and Delone model in 1992 as well as Pitt's model back in 1995. This new model is not similar to the past models. The difference exists as follow: (a) the service quality was added, (b) a workgroup was added to assume the external and organizational context related to the approach of contingency (Figure 2.5).

Figure 4: Myers, Kuppelman, and Prybuton (1997)



After over a decade past, McLean and Delone provided a model in 2003 that was updated and it disclosed the other researcher's criticism as well as the situation of that time. When the concept of service was added to information technology, the number of IS success elements were increased by means of using internet as well; moreover, it accelerated to seven and contained quality of service alongside with the interrelation and the correlation of them that were analyzed

Figure 5: Delone and Mclean IS success model (2003)

(Figure 2.6).

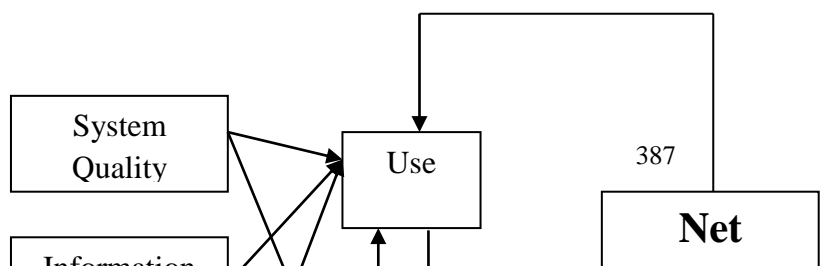
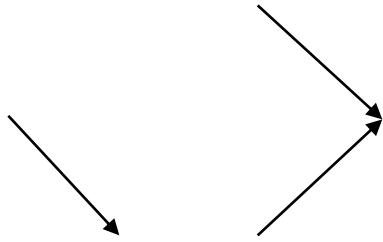


Figure 3: Pitt, Watson, And Kawan success model (1995)



According to the results from previous researches many empirical studies support the left side of the model by McLean and DeLone which states that information quality, system quality and as well as service quality lead to user satisfaction and system usage. It was clarified that the manner and attitude can be influenced by quality in the context of IS. But there still exist some arguments about information system success construct.

This construct is different in accordance with the domain. The success model of IS in a lot of various industries have been used such as construction, and the experts that tried to set up and apply a success model of IS that started to appear and some of them have been conducted. The studies related to this topic of construction contain the following aspects. (a) based on the model presented by McLean and DeLone they attempted to determine the factors of the success or the fault of the ERP system introduction that are utilized significantly in enterprise construction with the aim of evaluation, plan and project conduction for setting up and introducing the Enterprise Resource Planning (ERP) in the enterprise.

In this study the elements of success for the ERP system are classified in two separated groups. The first one is variables that are related to users like job relevance, output, result, image, system reliability and compatibility. The second group is variables that are related to the project which contain function, internal support and the support of consultant.

It can be concluded that the degree of completion for this research is high; furthermore, it offers a model of success to build the ERP system by a huge collection of data process as well as the data analysis. On the other hand, it should be mentioned that the recommended model has some restrictions for application for other types of IS due to the fact that it was described by concentration on ERP systems.

(b) The elements related to attitude and behavior of end users were analyzed by EDM which is the management and engineering system which is for projects that have a large scale construction (Hjelt et al., 2007). The study provided a survey in which the elements that affect the Electronic Document Management (EDM) system acceptance will be drawn for a project that is constructive.

Based on these elements, the IS success model that was improved by McLean and DeLone mentioned that the function where an end user agrees with an EDM system in a project that is constructive. (c) Related to the above researches (Raymond et al., 2008) offered a model of success for project management information system or PMIS in accordance with the IS model of success and the rest of the theories. Based on this study the important elements that influence the success of PMIS are the information quality of PMIS and quality of PMIS.

To assess the quality of PMIS, it was decided to use eight items which are response time, accessibility, ease of use, flexibility, learning ease, querying ease, multi project capability and system integration. There are six factors for estimation of information quality of PMIS which are relevance, availability, precision, reliability, security and comprehensiveness. However, as the authors declared the biggest flaw in this research is the fact that the model was measured by a small sample size which has been about 39 individuals. The most related investigations provided a success model of IS based on the model of McLean and DeLone.

The goal of this research is recommending a model of IS success that is developed according to the two available models. Therefore, the recommended IS model of this study will depend to green products and services usage in industry of education.

2.4 Green Environment in Malaysia

The application of green products is same to green purchase and the reason is because the goal for both of them is the similar as the other one. Green purchasing can be expected as a crucial tool for replacement of environment; in addition, the friendly usage as well as behavior of the production and consumption that provides a frequent green, and has many issues dependent to the environment like CO₂ emission reduction.

The sectors all around the world including private, public or social were asked to purchase green to have a stable future (IGPN, 2009). Malaysia in terms of quality of marines and rivers have a normal level and range. From 146 rivers, 7 of them have been monitored, it means that around 4.8% of these rivers have been categorized as polluted. This number of polluted rivers is more related to the amount of unhealthy rivers back in 2005 that was 10.3% or 15 rivers, but due to the fact that there was mist from July to October in 2006. While comparing with the past year the air had a fall down related to quality (Department of Environment, 2006).

The amount of waste had an increase from 548,916,11 metric tons back in 2005 up to 1,103,457,06 metric tons in the next year. From the different sources that bring a polluted air, three sources are from the vehicles, some of the industries like powerstations as well as operations which were negligent regarding an open burning in the country (Department of environment, 2006).

The main categories of waste produced in Malaysia which are hydrocarbon and oil, mineral sludge, dross, heavy metal sludge, gypsum and finally e-waste. Quantity of scheduled wastes generated by industry ranked from chemicals (42.7%), electronic (21.6%), automotive/workshop (17.2%), metal (7.1%), pharmaceutical (2.9%) and other industries (Department of environment, 2006). It is anticipated if this trend of irresponsible behavior and consumption patterns continue, the environmental degradation would be aggravated. Therefore a shift towards green products and processes is required.

If the process of increase in economy and as well as using the patterns in a negligent way remains, there will be a vast damage on environment and ecosystem in Malaysia. The concept of green purchasing is new in Malaysia (MGPN, 2003). Until now, there have been little inquiry on doing the green purchasing for individuals in Malaysia. However, it can be mentioned that big organizations that are located in United States (US) or United Kingdom (UK) and other countries in Europe are developing some go green campaigns for advancing this concept.

On the other hand, the local industries do not care to this aspect; furthermore, they always wait to see what will happen (MGPN, 2003). The Green Purchasing Network Malaysia (MGPN) president during his speech in the first International Conference related to the green purchasing expressed that it is better that the government establish a condition to motivate firms to be the initiative and first leader for green buying performance.

2.2 System Quality

Generally, the quality of system compared to quality of information achieved a lower level of attention in the literature of IS. Additionally, the system quality factors are usually related to aspects related to ease of use and quality of service. For example (Bailey et al., 1983) contained several various system concepts related to services of IS in their investigations of satisfaction. (Raiet, 2002) expressed that system quality can be evaluated by operation of ease of use. These aspects are entirely related to each other but they are not similar.

An easy to use system can be also high quality so the easy usage of a system can be the result of quality of system. Furthermore, systems bundled with a high level of IT service may be considered to be of higher quality, making service quality a covariate to the quality of the system.

The above relations are the results of models of system success (Seddon et al, 1997). It brings a situation which expressed it is essential to make sure about the conceptual clarification for the distinction and specification of the aspects. In this case our offer is that there exist some dimensions which are unique that are the important parts of the system quality and they act separately from service elements or ease of use.

The degree in which quality of information has a relationship with output of the information system and the quality of system shows the needed system of information process for making the output. So the system quality dimensions demonstrate perception of users for interacting with the system during the time. In this case systems with more quality can be assumed as more easy to use and also have more usefulness in usage (Davis, 1989).

The interaction of system in an organizational environment happens with the aim of doing a defined task most of the time. Hence it will be better to assume the aspects of system quality by means of spectrum which has a ranking from system to task. Dimensions of a system can be described as the characteristics of a system which is essentially differs in various uses and can be measured independently from the task, application or the environment. The dimensions of a task can be defined as the elements of evaluation which are related to setting and task.

Our understanding of past studies demonstrates that there exist five necessary dimensions for the quality of system which are reliability, accessibility, response time, flexibility and finally integration by conducting more than 20 investigations for recognizing the system quality aspects.

2.3 Information Quality

The goal of developing information systems is bringing valuable information for decision making for the groups and individuals by management of sources, processing, storage and keeping. Their real value and benefits will be known while the provided information will be used in operations. (Swanson, 1974) expressed that quality of information that shows the degree of information system success is an important factor.

The concept of information quality demonstrates the output quality which is produced by information system (DeLone et al., 1992). This can be a report or an online screen. In 1987, Pazer and Ballou presented four dimensions for the quality of information including completeness, accuracy, timelines and consistency. There are also some aspects for data quality. (Nelson et al., 2005) decided to apply the accuracy, construct, currency, and completeness and information quality format. Based on these researchers format, an extra construct have been used in relation with layout presentation for the output of the information.

The concept of accuracy usually expressed as the degree of correctness in stored information's mapping process for a proper state in the real context which the information demonstrates (Delone et al., 2003; Zmud, 1979; Nelson et al., 2005; Narasimhaiah et al., 2010; Fisher et al., 2001). When completeness mentioned, it is meant that the benefits and values of a defined variables have been recorded. It focuses on the fact that whether all values for all the factors have been recorded and kept. (Zmud, 1979; Nelson et al., 2005; Narasimhaiah et al., 2010; Fisher et al., 2001).

The term consistency demonstrates the data value has the same representation in all of the situations (Ballou et al., 1987; Pallant 2001, Hair et al. 1998; Nelson et al. 2005). On the other hand, currency means the extent in which there exists updated information and the degree of power of information to reveal the current situation that is reflected around us globally. Additionally, timeliness means that there will be no out of date value.

It is essential to have a data that is always available to influence the decision making and as a result, it can be changed in accordance with context and the person who makes decision. For instance a strategic developer might apply the information that is not new, but a production manager must have the latest updated data (Delone et al., 2003; Zmud, 1979; Strong et al., 1996). According to DeLone 2003, representative quality shows the format (Barki et al., 1985; Nelson et al., 2005). In fact when the word format is used, it means that the extent in which the presented information acts in a way which can be understood and explained for users, and also helps the task to be completed.

The relevance of the data describes the data application for a defined problem by a defined user. Related data can be used in a direct way to solve business problems (Ballou et al., 1987). Table 2.1, shows five main groups of information quality which are currency, format, dimension completeness and accuracy.

Dimension	Definition	Information quality category
Accuracy	The degree in which information is correct, meaningful, believable, and consistent.	Intrinsic
Completeness	The degree in which all possible states relevant to the user population are represented in the stored information.	Extrinsic; contextual
Currency	The degree to which information is up-to-date, the information precisely reflects the current state of the world that it represents.	
Format	The degree to which is presented in a manner that is understandable and interpretable to the user and thus aids in the completion of a task.	Extrinsic; representational

2.4 User Satisfaction

The positive effect of user satisfaction on performance of individuals was supported in past studies (Gatian et al., 1994; Guimaraes et al., 1997; Igbaria et al., 1997). For example the survey related to server/client system that was developed by (Guimaraes et al., 1997) it was found that the satisfaction of end users influences positively end user's job (the accuracy that is requested by job, feedback on job performance and skills required for the job). According to statement developed by (Igbaria et al., 1997) the satisfaction of users is considered as a factor which has the most powerful effect that is also direct on people's assumed impacts of performance, but is recognized a significant role for using the system for moderating the individual impact and the relation with user satisfaction.

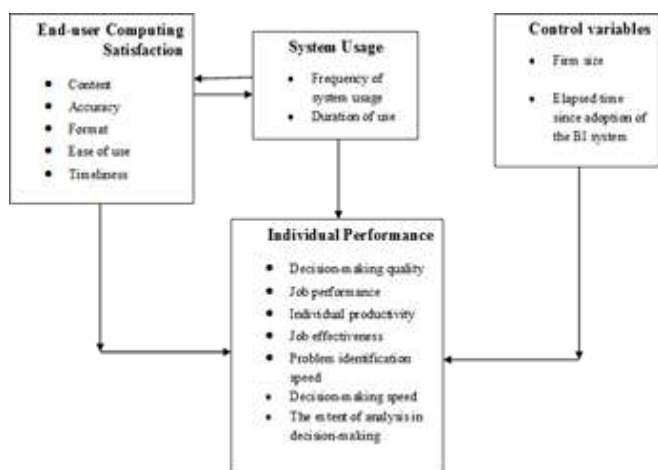
Besides, other experts recommended that the degree of individual impact will alter by user satisfaction for example effectiveness of performance, decision, understanding the information, identification of problem and the individual productivity.

The main objective of (Hou, 2012) in his research was testing the framework for comprehension of the relation between system usage, EUCS or end user computing satisfaction and also individual performance. Data was collected from 330 end users in BI or business intelligent system in electronic industry of Taiwan that was used to measure the recommended relation in the framework by means of structural equation of the method of modeling. This model was received strong support by the result which has been collected. The results demonstrated that the usage of BI

Table 1: Four broad categories for information quality(Ballou and Pazer 1987)

system as well as performance of individual can be enhanced by having more EUCS. (Figure 2.7).

Figure 5: Impact of user satisfaction on individual performance



2.5 Trust

As Manafi et al. (2011) cited, Lee and Fung (1999) and Fukuyama (1995) trust is defined as the willingness and thoughts about relying on someone's goodness, strength and fairness. Of the internet in this regard could be a good example. Sloman & Grandison conducted other research in 2000, and described trust as the idea of one firm to do individually and dependently with a specific meaning. They defined trust based on behavioral and security issues, while popularity and reliability of trust suggested by Fukuyama.

2.6 Trust and User Satisfaction

User satisfaction is a popular measure of IS success, in which many standardized instruments have been improved and tested (Zviran et al., 2003; Doll et al., 2004). User satisfaction is an essential construct because it's related to other important variables, including systems analysis and design. Satisfaction has been used to evaluate IS success and effectiveness, the success in decision supports systems, office automation success and the utility of IS in decision making (Zviran et al., 2006). In web-based systems, specially, satisfaction can depend on multiple factors, such as content, navigation, information structure, user interface and web design.

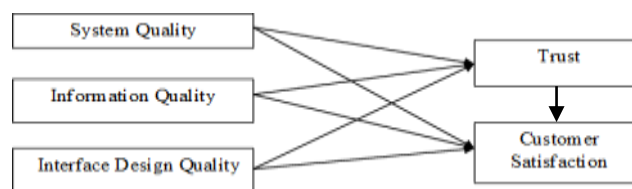
Satisfaction greatly depends on performance from marketing perspective; however, product experience does not define overall satisfaction lonely (Anderson et al., 1993). Research has described that the expected performance level and knowledge achieved by outcomes that were not experienced are also important. In other words, when individuals measure outcomes, in fact they compare their experienced results with

the results that might have occurred and chosen differently (Kahneman et al., 1986).

In a similar manner, development of trust has been described as the process setting expectations of another's behavior and then measuring whether those expectations have been confirmed (Garbarino et al., 1999).

Expectations can act as cognitive filtering devices by predisposing one individual to interpret another's behavior as consistent with original expectations. For instance, Holmes (1991) understood that trusting marriage partners block out or reinterpreted actions by their spouse positively that didn't match their trusting expectations. In this regard, when a consumer trusts an institution, it means there are expectations for satisfaction according to the institution's website that are likely to be confirmed. Beside as shown in Figure 2.8, user satisfaction extended to customer satisfaction and tested following framework in mobile banking industry (Lee and Chung, 2009).

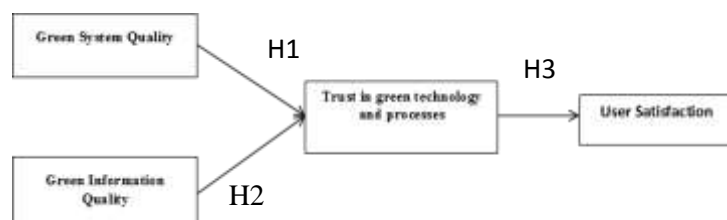
Figure 6: Lee and Chung 2009



2.7 Hypotheses development

By reviewing and getting knowledge from previous studies and investigations, this current study recommends a framework. With no doubt all of the links in this framework are supported by the past studies (Figure 2.9).

Figure 7: Proposed Framework



It is crucial to evaluate the impact of independent factors on dependent factors. It can be done after defining the theoretical model as well as independent factors. So there are five formulated hypotheses as the following statements:

H1: Trust is affected by system quality positively and significantly.

H2: Trust is affected by information quality positively and significantly.

H3: user satisfaction is affected by trust positively and significantly.

3. Method and results

To test mentioned hypotheses, this research applied quantitative approach. In this regard, the questionnaire was adapted from prior research developed by Delone and Mclean (2003) and Lee and Chung (2009). It should be mentioned that all items of questionnaire were based 5-point Likert scale. The staffs who are working at University Putra Malaysia (UPM) are considered as the population of this study. They will be selected between the official members because they are more participating in internal process that is non paperless or paperless. Besides, the sample size was 150. Table 2 shows the frequencies of demographic questions.

Table 2: Frequency of demographic questions

		Frequency	Percent	Valid Percent	Cumulative Percent
Age					
Valid	less than 20	30	20.0	20.0	20.0
	21-40	54	36.0	36.0	56.0
	41-50	42	28.0	28.0	84.0
	more than 51	24	16.0	16.0	100.0
	Total	150	100.0	100.0	
Gender					
Valid	Male	84	56.0	56.0	56.0
	Female	66	44.0	44.0	100.0
	Total	150	100.0	100.0	
Educational level					
Valid	high school and Diploma	45	30.0	30.0	30.0
	Bachelor	81	54.0	54.0	84.0
	master or higher	24	16.0	16.0	100.0
	Total	150	100.0	100.0	

Besides, Table 2 represents central indicators of each item of questionnaire.

Table 3: Measure of the Construct and descriptive

Constructs	Mean	Standard Deviation	Kurtosis	Skewness
Green System Quality				
The green technologies (e.g. paperless process, faster PCs, latest version of windows, disposable glass, etc.) can be applied in my job.	3.5533	1.27725	-.698	-.505
The green technologies/products can be considered as reliable in my job.	3.6867	1.05000	-.188	-1.172
I have access to green products/processes any time I need.	3.4067	1.14749	-.497	-.458
The green products and processes are usable in my job.	3.6867	1.05000	-.188	-1.172
Green technology facilitates my job as well as other technologies are being used.	3.5200	1.40813	-.633	-.882
Green Information Quality				
By using the green proceeding (online banking, e-filing of taxes, etc.) can support all means of information and services.	3.3200	1.15462	-.546	-.857
In green process, everything is more understandable.	3.4067	1.14749	-.497	-.458
The green services can connect internal and external Networks	3.0467	1.29706	-.387	-1.089
I think the green services makes a company's activities as secure as well as other working processes like bookkeeping, sales tracking, etc.	3.0733	1.25370	-.161	-1.192
Trust				
I really think by using green products at the university affects positively the environment.	3.4000	1.56728	-.369	-1.384
I really think by using green processes at the university affects positively the environment	3.3000	1.00835	-.036	-1.247
Using the green technology enhances my effectiveness in my job.	3.1000	1.30436	-.463	-1.033
Using green technology (product and process) facilitates the internal process towards a green environment.	3.1000	1.22474	-.193	-1.222
User Satisfaction				
The green technology provides the precise information I need.	3.3800	1.51356	-.373	-1.265
The information content provided by the green technology meets my need.	3.4133	1.02444	-.104	-1.180
The green technology provides reports that seem to be just about exactly what I need.	3.1000	1.30436	-.463	-1.033
The green technology provides sufficient information.	3.2533	1.14802	-.430	-.943
Using green process/technology is pleasant for me.	3.2800	1.26978	-.243	-.825

The results of reliability test shows all values more than .07. It means that all of the variables have acceptable internal consistencies (Nunally, 1978).

Table 3 shows the results of Pearson correlation test. It can be sure that the connection and relationship among each two elements is positive because all of the p-values are below 0.05. Also, all of the correlations are seen as positive that shows the relationship is positive. From the information quality and system quality, the maximum correlation related to information quality (.742). Besides, the relationship between trust and user satisfaction is positive and significant because p-value is zero and estimated correlation is .794.

Table 3: Correlations

		System Quality	Information Quality	Trust	User Satisfaction
System Quality	Pearson Correlation	1	.795**	.615**	.464**
	Sig. (2-tailed)		.000	.000	.000
Information Quality	Pearson Correlation	.795**	1	.742**	.526**
	Sig. (2-tailed)	.000		.000	.000
Trust	Pearson Correlation	.615**	.742**	1	.794**
	Sig. (2-tailed)	.000	.000		.000
User Satisfaction	Pearson Correlation	.464**	.526**	.794**	1
	Sig. (2-tailed)	.000	.000	.000	

Referring to the proposed framework of this research, two regression analysis were applied. The first regression analysis refers to the impact of information quality and system quality on trust. The second analysis measured the impact of trust on user satisfaction. According to the first regression analysis' results, R square is equal to .553. This shows the fact that 55.3% of variation related to trust can explained by information quality and system quality. By using the Analysis of Variance (ANOVA) table, at least one of the variables has significant impact on trust because the p-value is equal zero. Besides, there is no multi co-linearity between information quality and system quality because Variance Inflation Factor (VIF) column shows value less than 5. (Hair et al. 2010).

The system quality has a significant and positive effect on trust because p-value is .022 (less than .05). The estimated coefficient is .172 that explains the positive influence. So, for

every unit increase in system quality, trust will go up .172 units. Hence, the first hypothesis is accepted by this study. The results obtained from this study is consistent with previous researches conducted by Delon and Mclean (1992), Vance et al., (2008), and Lee and Chung (2009).

The information quality also has a significant and positive effect on trust because p-value is zero (less than .05). The estimated coefficient is .798 that explains the positive influence. So, for every unit increase in information quality, trust will go up .798 units. Hence, the second hypothesis is accepted by this study. The results obtained from this study is consistent with previous research conducted by Delon and Mclean (1992; 2003), and Aberer et al., (2001). However, the final regression equation is as below:

$$\text{Trust} = .403 + .172 (\text{system quality}) + .798 (\text{information quality})$$

In the second regression analysis, R square is equal to .631. This shows the fact that 63.1% of variation related to user satisfaction can explained by Trust. By using the ANOVA table, the user satisfaction will be affected by the trust because the p-value that is 0.00 and less than 0.05.

The trust significantly impacts on user satisfaction because p-value is 0.00. The estimated coefficient is .710 that explains the positive influence. For every unit increase in trust, user satisfaction will go up .710 units. So, the third hypothesis is supported by this study. The results obtained from this study is consistent with the previous researches conducted by famous scholars for instance Bouckaert et al., (2003), and Morris et al., (2002).

However, the final regression equation is as below:

$$\text{User satisfaction} = .994 + .710 (\text{Trust})$$

Recommendation, Limitation, and Future Study

According to results of this study, Green system quality, Green information quality have significant and positive impacts on Trust, in addition, Trust has a significant and positive impact on user satisfaction. Hence, every effort on planning, promotion, and improvement in System quality, Information quality will help to trust among university staff.

On the other hand, every effort on trust will lead to user satisfaction in the studied university. Therefore, from the mentioned practices, having a clear policy and rules for promotion of quality factors leads to trust thereby user satisfaction among staff.

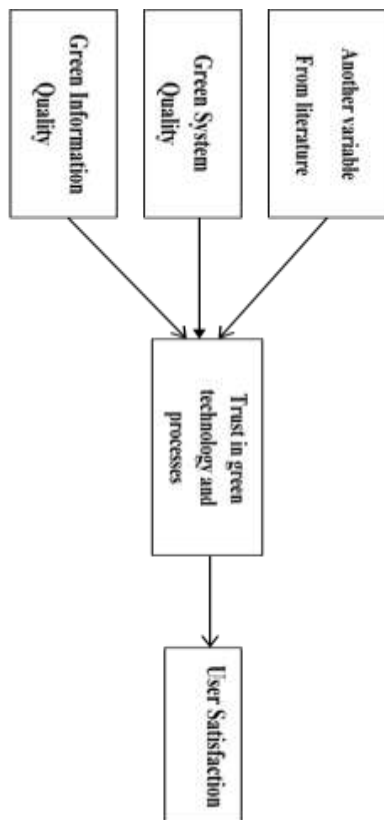
The most important limitation for this study is data collection from participants because some of the university staff had a

little familiarity with green technology and processes, for example, what kind of tasks can help to green environment at the university. On the other hand, tendency of some staff showed little willingness to participate, and also some of them thought that participation in this research may be contradictory with the policy of the university.

As suggestions for future researches, this study recommends that proposed framework used in this study is examined at other universities. Besides, researches similar to this study can be conducted in industries such as manufacturing or banking.

Furthermore, R-square in the first Multiple Regression analysis is .553 although this value is not very low, but it motivates that in future researches a new variable is identified according to literature review to help improve the framework used in this study.

Figure 8: Proposed Framework for future study



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Energy Loss Estimation and Flow Simulation in the skimming flow Regime of Stepped Spillways with Inclined Steps and End Sill: A Numerical Model

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Abstract: Energy dissipaters in dams consider as expensive structures; therefore, economic design of these structure are desirable. Stepped spillways can be use as energy dissipater to reduce the size and cost of the stilling basin. Hard experimental works, high-cost and time-consuming laboratory methods brought about some difficulties to determine the most-efficient design of the steps. This research deals with comparing the two-dimensional numerical simulation and experimental description in stepped spillways equipped with inclined steps and end sill together and presents a quick, trustworthy, economical, and numerical approach to designing the steps. In complicated geometries, simulation is more problematic than simulation of flow in horizontal steps, because it needs more precision around the end sills. Finite volume method and the k- ϵ standard model are proposed to simulate the flow pattern and evaluate the energy loss over stepped spillway. The flow pattern and velocity vectors resulted from numerical simulation is in a good agreement with the experimental results. Also, energy losses resulted from the numerical approach have been compared with laboratory measurements and demonstrate reasonable agreement.

Keywords: stepped spillway; energy dissipation; inclined steps together with end sill; finite volume method; and k- ϵ standard model; skimming flow regime

1. INTRODUCTION

Subgrade support system has a great influence on structures' behavior [1] [2]. Water flow from dam can damage downstream structures and expedite deterioration of their support system so a dissipate flow energy system is crucial to dams structural design. Dissipating energy over the chute may reduce the size of the stilling basin. In recent decades, several studies have addressed different aspects of stepped spillways; these studies have also introduced them as an efficient energy dissipater [3][4]. Three flow regimes can be seen over stepped chutes based on discharge rate. In the low-rate flows, Nappe flow regime is observed; and the Skimming Flow is caused by high discharge rates and between these two flow regimes Transition flow regime can be seen [3][4]. Chamani and Rajaratnam also Chanson Performed experiments on the Skimming Flow regime and devolved experimental formulas to determine the energy loss rate in this regime [5][6]. Some efforts has been made to use numerical simulation and machine learning in engineering [7] [8]. Chen et al. used finite volume method and utilized the k- ϵ turbulent model to determine flow turbulence in stepped spillways [9]. Tabbara et al. simulated the flow over stepped spillway by the finite element method using ADINA software with the k- ϵ standard turbulence model [10]. Mousavi-Jahromi et al. used ANSYS software to simulate the flow over stepped spillway [11]. They reported that numerical results have a six percent differential with experimental ones. The K- ϵ model was initially formulated by Spalding and Launder [12]. Two equations for the k- ϵ turbulence model have been recognized as the appropriate formulas to simulate spillway flow. Other works have been conducted on flow condition, aeration, and energy loss in stepped spillways with horizontal steps. Boes and Hager [13], Cheng et al. [14], Estrella et al. [15] considered velocity and air concentration in air-water flow. Felder et al. did experimental study regarding air-water flow properties and energy dissipation [16], Gonzalez studied on free surface aeration [17], Ohtsu and Yasuda considered characteristics of flow conditions on stepped channels [18],

Toomes investigated air-water flow properties on low gradient stepped chutes [19], Zare and Doering worked on inception point of air entrainment and energy dissipation when stepped spillway equipped to baffles and sills [20] [21].

Moreover, other works on flow condition, and energy dissipation in stepped spillways equipped with inclined steps or an end sill, have been conducted and the results indicate that inclined steps are reduced more energy than horizontal steps [22] [23] [24] [25]. Among all the investigations conducted on spillways, the research performed by Chaturabul can be singled out [24]. In his research, the height of the applied end sills was considered at 5, 10, and 15 millimeters on various step slopes. The result of his investigation demonstrated that due to the existence of an end sill, relative energy loss increased 8%. Chinnarasri and Wongwises examined inclined steps and the end sill to determine the energy dissipation rate independently [26]. They reported that using an end sill is the best method to increase the energy dissipation rate. As mentioned before, some researcher simulated flow over stepped spillways with horizontal steps, but no one had tried to simulate flow over stepped spillway equipped with inclined steps and an end sill together. In this kind of chutes, simulation is more difficult than horizontal steps, because more accuracy is needed accuracy around the end sills. In this paper, the finite volume method and the k- ϵ turbulence model in FLUENT 6.3 have been utilized in two-dimensional mode to estimate the energy loss also simulate the flow pattern, find velocity vectors and flow direction over a stepped spillway equipped with inclined steps with an end sill together. Flow depth and velocity are calculated numerically in specified sections, and energy loss is computed at each of these sections. Dimensionless parameters are used in this research to show the effectiveness of height and thickness of end sills on energy loss rate also experimental set up and results are presented then in the numerical part of the research, reasons to select grid type, boundary condition type and turbulence model are discussed. In the end, the effectiveness of the proposed numerical model to simulate the

flow pattern, velocity vectors, flow direction and evaluate energy loss rate in a stepped spillway equipped with inclined steps with an end sill are discussed.

1.1 Energy Loss Equations

Chanson presented an equation in order to estimate dissipation energy rate in Skimming flow in stepped spillways [6]:

$$\frac{\Delta H}{H_{max}} = 1 - \frac{\left(\frac{f}{8 \sin \theta}\right)^{\frac{1}{3}} \cos \theta + \frac{1}{2} \left(\frac{f}{8 \sin \theta}\right)^{-\frac{2}{3}}}{\frac{H_D}{h_c} + \frac{3}{2}} \quad (1)$$

Where f can be obtained as follows:

$$\frac{1}{\sqrt{f}} = 2.43 - 0.2676 \ln \left(\frac{h_s \cos \theta}{D_H} \right) \quad (2)$$

Where D_H is hydraulic depth of flow. Foregoing equation is applicable for mild slope chutes ($\theta \leq 20^\circ$). Another equation, which can be used for determining the dissipation energy rate in the Skimming flow regime, is the utilization of Chanson's equation to calculate the remaining energy at the end of the chute. [6]

$$H_{res} = y \cos \theta + \frac{q^2}{2gy^2} + z \quad (3)$$

Where y is depth of fresh water and H_{res} is remaining energy at the end of the chute. The following equation is to calculate y:

$$\frac{y}{h_c} = \sqrt[3]{\frac{f}{8 \sin \theta}} \quad (4)$$

f is calculated from (2). The following equation has been also offered by Chamani and Rajaratnam in order to estimate the remaining energy at the end of the chute. [5]

$$H_{res} = y_m \cos \theta + \frac{u_m^2}{2g} + z \quad (5)$$

Where y_m is mixed depth (air and water); u_m is mixed flow velocity and z is height from baseline.

2. DIMENSIONAL ANALYSIS

Buckingham's Pi Method, as one of the most appropriate methods in dimensional analysis, has been used in this study. Effective parameters for energy dissipation in sloped stepped spillways, include: discharge per unit width, flow head, step length, step height, slope height, and gravity acceleration [27]. In this research, other factors such as spillway slope, water density and number of steps are considered as follows. Effective factors for energy dissipation in a stepped spillway equipped with inclined steps and the end sill together include:

q: Discharge in the unit width of the spillway

s: The spillway slope

E_L : Energy loss

E_0 : Flow head

h: Step height

ρ_w : Water density

l: Step length

N: Number of steps

m: Height of (slope + end sill)

t: Thickness of the end sill

g: Gravity acceleration

$$E_L = E_L(q, E_0, h, l, m, t, g, s, \rho_w, N) \quad (6)$$

Dimensionless parameters resulted from Buckingham's Pi theories:

$$f = f(E_L, q, E_0, h, l, m, t, g, s, \rho_w, N) \quad (7)$$

The number of variables is $n=11$.

$$\rho [ML^{-3}], g [LT^{-2}], h [L] m = 3 \rightarrow \text{Basic dimensions}$$

$$\pi = n - m = 11 - 3 = 8$$

$$f(E_L, E_0 h^{-1}, q \sqrt{\frac{1}{g h^3}}, l h^{-1}, m h^{-1}, t h^{-1}, s, N) = 0 \quad (8)$$

$$\varphi \left(\frac{E_0}{h}, q \sqrt{\frac{1}{g h^3}}, \frac{l}{h}, \frac{m}{h}, \frac{t}{h}, s, N \right) = 0 = E_L \quad (9)$$

The performed dimensional analysis is for a stepped spillway equipped with inclined steps and the end sill together. In this research, only the "m/h" dimensionless parameter is used.

3. EXPERIMENTAL SETUP

This research has been conducted at the Water Research Institute in Iran. Side walls and steps were made of Plexiglas. The broad-crested weir has been used as the spillway in the chute and the number of steps is 60. In the present investigation, only four steps are inclined and equipped with the sill; all are placed after the middle of the chute (steps 39-42). The horizontal length of the steps is 14 centimeters; the step height is 4.66 centimeters and the chute width is 1.33 meters. Flow depth and velocity have been measured during each test using a liminimeter (with a precision of 1 millimeter) and a pitot-tube, respectively. The experiments have been conducted for one discharge in the Skimming Flow regime (90 liters per second, $q=0.0677 \text{ m}^2/\text{s}$). Flow discharge has been measured by the sharp crested weir at the end of the downstream chute. Characteristics of the used end sills are presented in Figure 1 and Table 1. Three different slopes of 7° , 10° , and 12° , respectively, about the horizon were used.

Table 1. End sill specifications

(p-t) mm	
6-5	6-10
8-5	8-10
10-5	10-10
15-5	15-10

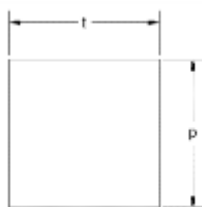


Figure 1. Schematic of the end sill

The depth along the spillway width was measured by a liminimeter across each line of the piezometers. Three depth measurement were recorded in each section because of insufficient liminimeter accuracy and the possibility of an outlook error. Finally, an average of these three depths across each line of the piezometer was used as the step depth. The pitot-tube was used to measure the velocity. This measurement was laborious, since the flow was a two-phase flow and bleeding had to be performed regularly. The velocity was measured on both sides and in the middle at 0.6 meters of depth. Finally, averages of these all three sections were averaged and set as the average velocity of that step. The piezometer was used to statically measure pressure fluctuation. These data points were used to enter pressures as initial values in a numerical simulation. In this chute, only four steps (39-42) were inclined and had sill. Depth and velocity values were measured on these steps, as well as on the 38th step.

The entrance flow from the reservoir into the chute flows through the transferring pipes from the pumps and falls into the reservoir. When the reservoir completely fills, the vent opens and flow falls into the chute. The utilized pump has a capacity of 220 liters per second. The following equations were used to determine upstream and downstream energy for the modified steps:

$$H_1 = y_1 + \frac{V_1^2}{2g} + z \quad (10)$$

$$H_2 = y_2 + \frac{V_2^2}{2g} + z \quad (11)$$

Where H is flow energy, y is flow depth, V is flow velocity in the proper sections, g is gravity acceleration and Z is the height above the baseline (The bottom of the last modified step has been assumed to be the baseline, and $Z=0$).

4. A NUMERICAL APPROACH

The numerical approach (Fluent 6.3) has been applied to simulate flow and estimate energy loss over stepped spillway equipped with an inclined step and an end sill, together. In this section, grid characteristics, the grid adaption method, boundary conditions, the turbulent model and the solver method details are discussed.

4.1 Geometry and Meshing

In the Finite Volume Method initial differential equations should be integrated into a physical space, and then should be solved using numerical methods. For that reason, point's grid should be developed directly in a physical space. Due to this, there is a non-zero probability that points in the grid don't relate to lines in the grid. These kind of grids are known as unstructured grids. A structured grid is easy to develop in simple geometry [28]. It needs less memory and time to resolve. However, in complex geometry, like the situation in this study, it is recommended to use unstructured grids with triangular elements. The required time to develop an unstructured grid in this study (complex geometry) is less than the required time to develop a structured grid. Although an unstructured grid needs more time and memory to solve the problem, it is still worth it to use in the study. The unstructured grid for this research was developed in Gambit software by triangular elements [29][30][31].

The Region Adaption Technique has been applied in this study. This technique makes triangular elements smaller around end sills, to achieve high accuracy. The grid has been divided into small triangles, depending on the required precision, (Figure 2) and considered 0.001 up to 0.01 meters, Also, to increase grid quality, smoothing and swapping have been applied. Smoothing rearranges cells to improve grid quality. It is recommended to use smoothing based on skewness when triangular elements have been used (Fluent 6.3 user's guide). For that reason, smoothing based on skewness has been applied to decrease the grid's maximum skewness. This method tries to decrease the skewness in cells with the skewness higher than the maximum limit, which is 0.4 in this study, by rearranging the cells. Furthermore, face swapping has been used to the grid to increase quality. In triangle cells, the Delaunay Method has been applied to improve grid quality.

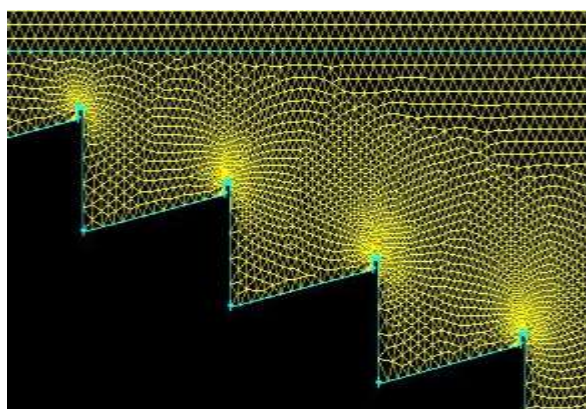


Figure 2. Applied unstructured grid

4.2 Initial and Boundary Condition

There are two sections in the inlet (Figure 3), which are separated by the flow surface. In the lower section, the boundary type has been selected as velocity inlet, because this part is full of water with a certain velocity. The flow depth in each test is selected as height of this section. Also, the velocity in each test is entered into the software by magnitude and direction. The x-direction is selected as a velocity direction. The second section is above flow, with the pressure equal to atmospheric pressure. For that reason, the pressure inlet boundary type is selected for this section. The area above the steps has a similar situation to the second section. Therefore, the pressure inlet boundary condition is selected for this area. In the outlet, there are two sections. The first section includes flow and the second one includes air. Because pressure inlet is selected in the inlet, the outflow boundary condition cannot be used in this section and the pressure outlet boundary condition should be used as boundary condition. In the end, the wall boundary condition has been applied to the steps.

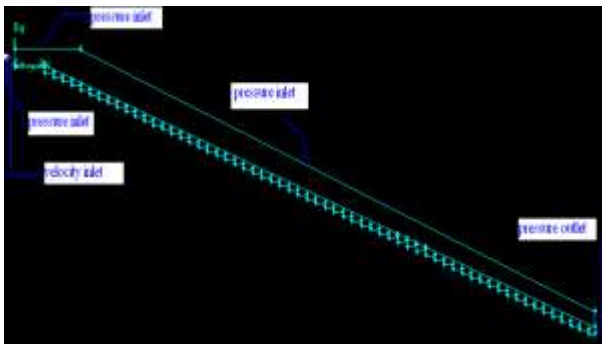


Figure 3. Boundary conditions

4.3 Turbulence Modeling

Both the water and air phases should be defined in the software to simulate the flow over the chute. The volume fraction is defined as “0” when the cell volume is out of water. The volume fraction is defined as “1” when the cell volume is full of water. The software will calculate the volume fraction of each cell based on the water and air percentage in that particular cell.

When the Reynolds number is large, or the geometry is complicated, it is impossible to solve time-dependent Navier-Stokes Equations completely. The Reynolds Average Navier-Stokes Equations (RANS) can solve the Navier – Stokes Equations in the way that turbulent flow fluctuations don't directly enter into the equations. In this method, new variables and extra quantities are introduced in governing equations. These new variables and quantities should be calculated by the turbulent models [30]. RANS Method has been applied in this research, because it can solve flows with a strong vortex and naturally unsteady flows with moderate cost. Among turbulent models, the Spalart- Allmaras, $k-\epsilon$, $k-\omega$, and Reynolds Stress Model (RSM) use the RANS Method and all of them are available in Fluent 6.3. In the RANS Method, continuity and momentum equations are as follows [33]:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0 \quad (12)$$

$$\begin{aligned} \frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_i u_j) = & \\ - \frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right) \right] & \\ + \frac{\partial}{\partial x_j} (-\rho \overline{u'_i u'_j}) & \end{aligned} \quad (13)$$

Where ρ is density, μ is molecular viscosity, t is time, x_i is the coordinate component, u_i is the velocity component, and p is pressure. Reynolds stresses should be calculated to solve the problem with the RANS Method. One of the methods that can be used to calculate Reynolds stresses is the Boussinesq Hypothesis (equation 14), which has a reasonable calculation cost.

$$-\rho \overline{u'_i u'_j} = \mu_t \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} (\rho k) \delta_{ij} \quad (14)$$

Where μ_t is the turbulence viscosity. $\delta_{ij} = 1$ when $i=j$ and $\delta_{ij} = 0$ when $i \neq j$. Some turbulent models like Spalart-Allmaras, $k-\epsilon$, and $k-\omega$ use the Boussinesq Hypothesis. The $k-\epsilon$ style models (standard, RNG, and Realizable) and the $k-\omega$ turbulent models solve two equations to calculate turbulent viscosity. The number of equations denotes the number of additional Partial Differential Equations (PDEs) that should be solved.

Among the $k-\epsilon$ style models (standard, RNG, and Realizable) and the $k-\omega$ turbulent models, the $k-\epsilon$ standard is selected to be considered in this study as the first turbulent model attempt, due to its simplicity and reasonable cost. Furthermore, it has been previously used to successfully simulate flow over stepped spillways [9]. This turbulent model solves “ k ” and “ ϵ ” equations as additional PDEs to find turbulent viscosity. “ $k(t)$ ” is an instantaneous kinetic energy and is the sum the mean kinetic energy (K) and the turbulent kinetic energy (k). k and ϵ (simplified) are as follows:

$$\begin{aligned} \frac{\partial (\rho k)}{\partial t} + \text{div}(\rho k U) = & \\ \text{div} \left[\left(\frac{\mu_t}{\sigma_k} \right) \text{grad} k \right] + 2\mu_t E_{ij} E_{ij} - \rho \epsilon & \end{aligned} \quad (15)$$

$$\begin{aligned} \frac{\partial (\rho \epsilon)}{\partial t} + \text{div}(\rho \epsilon U) = & \\ \text{div} \left[\left(\frac{\mu_t}{\sigma_\epsilon} \right) \text{grad} \epsilon \right] + C_{1\epsilon} \frac{\epsilon}{k} 2\mu_t E_{ij} E_{ij} & \\ - C_{2\epsilon} \rho \frac{\epsilon^2}{k} & \end{aligned} \quad (16)$$

There are five terms in both equations. From left to right, the terms are the rate of increase, convective transport, diffusive transport, the rate of production, and the rate of destruction, respectively. Where μ_t is calculated by the following equation using k and ε (turbulence energy dissipation rate):

$$\mu_t = \rho c_\mu \frac{k^2}{\varepsilon} \quad (17)$$

Where ρ is the fluid density, c_μ is the experimental constant and equals to 0.09. Prandtl's turbulence numbers for k and ε consist of $\sigma_k=1.0$, $\sigma_\varepsilon=1.3$, $C_{1\varepsilon}=1.44$ and $C_{2\varepsilon}=1.92$, which are the constants of the relation ε [34]. The Second Order Implicit pressure based solver has been applied in this research. Moreover, the segregated algorithm has been used, because it needs less memory than the coupled algorithm. Furthermore, the First Order Upwind Method has been applied in turbulent kinetic energy and turbulent dissipation rate equations. The PISO method has been applied as a pressure velocity coupling method.

5. RESULTS AND DISCUSSION

The energy loss outcomes from the horizontal steps was 0.3514 and 0.3508, respectively, derived from the Chanson equations (Equations 2 to 5) and from the test (Equations 10 and 11), which shows acceptable agreement. The changes were then applied to the steps, and the energy loss was measured for various slopes and end sills. In this section, the parameter $m = (p+w)$ is used, where p is the height of the end sill, and w is the height of the step inclination (Figure 4).

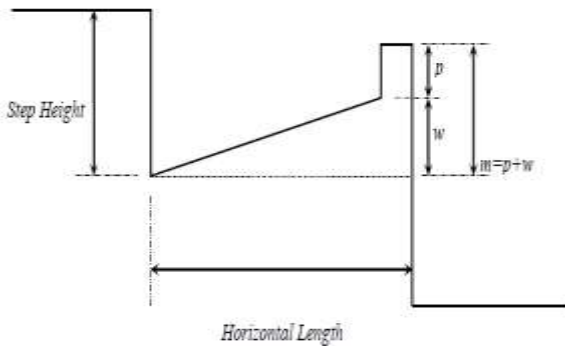


Figure 4. Schematic of the step

In Figure 5, it is obvious that if the “ m/h ” ratio increases, up to 0.7, the energy loss rate increases. After that, it decreases. This graph indicates that the best ratio for “ m/h ” is about 0.7, and an excessive increase negatively affects the energy loss rate. When the “ m/h ” ratio goes past 0.7, the flow jumps from one or more steps and the energy loss rate decrease (Figures 6a and 6b). This step plays practically no role in energy dissipation. As a consequence, the energy loss rate decreases.

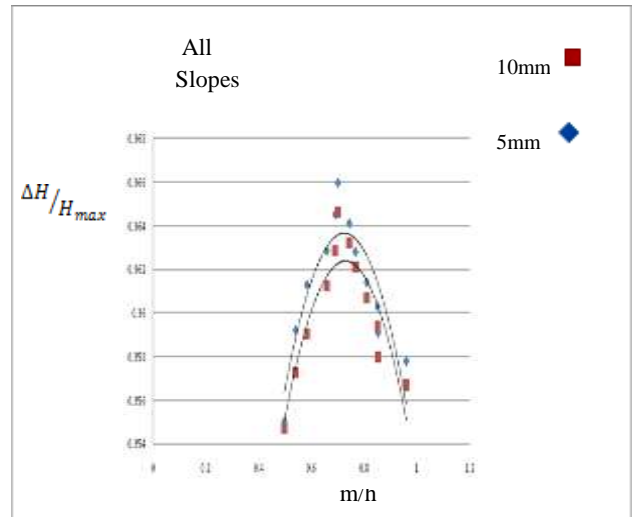


Figure 5. Energy dissipation loss per “m” for all examined slopes

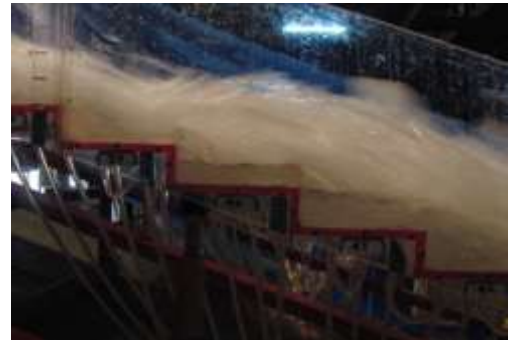


Figure 6a. Slope 7°, height of end sill=6mm and thickness=5mm



Figure 6b. Slope=12°, height of end sill=15mm and thickness=5mm

Table 2 presents the results for the inclined steps and end sills for the “ m/h ” equal to or greater than 0.7 (effective end sills). The outcomes indicate that the end sill height, as well as the step height incline (w), affect the energy dissipation rate slightly but thickness has no meaningful effect on energy loss rate. Table 2, also, indicates that “the maximum energy loss increase” is 4.13%, and “the average energy loss increase” is 2.74%. This amount of increase in the energy loss is not considerable and proves that step modification (inclined step and end sill) is not an effective technique to increase the stepped spillways’ efficiency in terms of energy dissipation in skimming flow regime.

Table 2. Comparison of energy losses derived from tests

Run#	Energy loss %	Thickness (mm)	m/h	Inclined step (degrees)	End sill Height (mm)	Energy loss%
1	35.50	5	0.50	7	6	1.18
2	35.92	5	0.54	7	8	2.39
3	36.12	5	0.50	7	10	2.88
4	36.28	5	0.66	10	6	3.31
5	36.45	5	0.69	7	15	3.76
6	36.59	5	0.70	10	8	4.13
7	35.47	10	0.50	7	6	1.10
8	35.72	10	0.54	7	8	1.79
9	35.90	10	0.58	7	10	2.28
1	36.12	10	0.66	10	6	2.96
1	36.28	10	0.69	7	15	3.31
1	36.46	10	0.70	10	8	3.78

Numerical analysis results are presented as velocity vectors and water surface profile (Figures 7a and 7b). As it can be seen in Figure 6a, after the flow encounters the end sill in the first modified step, it jumps from the second and the third modified step. During the jump, some parts of the flow can't reach the last modified step and fall into the second and the third steps. Due to reverse inclined shape of the steps, this flow will stay in the second and the third steps and make a deep pool. The flow direction in the pool is from the end sill to the wall (from right to left) due to the step slope. Other parts of the flow jump to the last modified step, and during the jump combine with air, making highly aerated flow over the chute. Figure 7a shows the flow profile simulation. This flow profile is the same as the flow profile obtained in the laboratory. Also, flow direction is illustrated in Figure 7b as velocity vectors. The flow direction is also similar to experimental results (Figure 7b). The velocity magnitude is larger in the jump flow and is smaller in the pool (Figure 7d). Experimental results confirm these values.

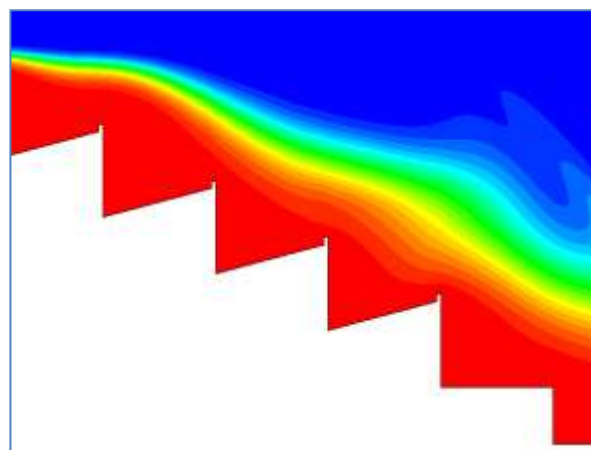


Figure 7a. Flow profile - Steep 10°- End sill 6-5 mm

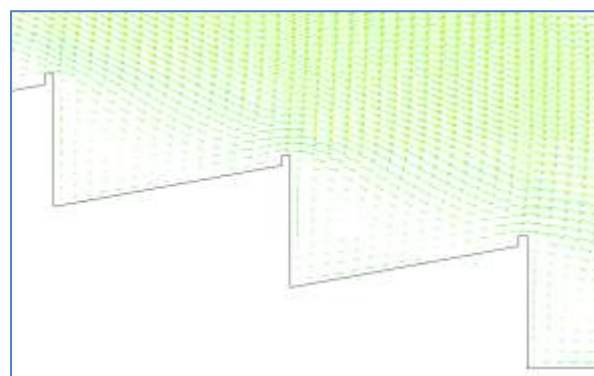


Figure 7b. Velocity vectors - Steep 10° – End sill 6-5 mm

Twelve tests have been performed in this research. The first eight tests are used for calibration, and other four tests are used for validation. In Table 3, there are eight tests which have been used to approach numerical calibration to simulate energy loss in the Skimming Flow regime. Moreover, the minimum error for calibration data is 5.37%, and the maximum error is 9.91%. Also, the average error for calibration data is 7.90%. Table 4 indicates numerical simulation results in which validation data have been applied. The minimum error for validation data is 5.44%, and the maximum error is 9.21%. Moreover, the average error for validation data is 7.61%.

Table 3. Energy loss -Various end sills –Calibration

Energy loss %			
Run#	Experimental	Numerical	Error%
1	35.50	37.78	6.03
2	35.92	37.96	5.37
4	36.28	38.99	6.95
5	36.45	39.18	6.97
7	35.47	39.37	9.91
8	35.72	39.58	9.75
10	36.12	39.79	9.22
12	36.46	40.06	8.99

Table 4. Energy loss – Varoious end sill - Validation

Energy loss%			
Run #	Experimental	Numerical	Error%
3	36.12	38.20	5.44
6	36.59	39.26	6.80
9	35.90	39.45	9.00
11	36.28	39.96	9.21

6. CONCLUSION

In this study, four steps (39 to 42) have been modified and equipped with inclined steps and an end sill, together. End sills with several heights and thickness have been tested in three reverse stepped slopes (7, 10 and 12 degrees, respectively). The “m/h,” has been used as a dimensionless parameter to determine the energy loss rate. Results denote that in the discharge 90 L/s ($q=0.0667 \text{ m}^2/\text{s}$), which represents the Skimming Flow regime, inclined steps and an end sill slightly increases the energy loss rate. The average of this increment is about 2.74% in effective end sills. Moreover, FLUENT 6.3 software was used in this research to simulate the flow over a stepped spillway. A numerical approach using the finite volume method, triangular elements, an unstructured grid and the k- ϵ standard turbulent model has been successfully applied to simulate flow pattern, velocity vectors in the complicated geometry of stepped spillways equipped with inclined steps and end sill together. Furthermore, the energy loss has been estimated using the numerical model. In the first step, eight tests (out of twelve) were selected for calibration; afterwards, four other tests were operated for validation. Numerical results for depth and velocity were used to calculate energy loss. The results illustrate some differences between the numerical and experimental

outcomes. Average errors, generated by comparing the energy loss results between the experimental and numerical methods, were 7.90% and 7.61% for the calibration and validation data, respectively. The amount of these errors denotes that numerical models can be used as a low-priced and prompt method to estimate the energy dissipation rate in a stepped spillway equipped with inclined steps and end sills together.

Acknowledgment

The authors wish to acknowledge the support received in the form of a graduate assistantship from the Civil and Environmental Engineering Department, Florida International University. Also, the authors wish to acknowledge the Water Research Institute, Iran for providing the model and instruments to conduct experiments in the hydraulic laboratory.

Notation

The following symbols are used in this paper:

- $C_{1\epsilon}$ = Constant in the k- ϵ turbulent model
- $C_{2\epsilon}$ = Constant in the k- ϵ turbulent model
- C_u = Constant in the k- ϵ turbulent model
- d_c = Critical depth (m)
- E_0 = Flow head (m)
- E_L = Energy loss
- H_1 = Total head in section 1 (m)
- H_2 = Total head in section 2 (m)
- h_c = Critical depth (m)
- H_{dam} = Dam height (m)
- H_{max} = Total energy ($H_{dam}+3/2h_c$) (m)
- H_r = Residual height (m) (Fratino and Piccini)
- h_s = Step height (cm)
- l_s = Horizontal step length (cm, m)
- u_i = Velocity component in the x-direction (m/s)
- u_j = Velocity component in the y-direction (m/s)
- u_k = Velocity component in the z-direction (m/s)
- $u'_{i,j}$ = Velocity component in the i- or j-direction (turbulent) (m/s)
- V_1 = Velocity in section 1 (m/s)
- V_2 = Velocity in section 2 (m/s)
- y_2 = Depth in section 2 (cm)
- ρ_w = Water Density (kg/m^3)
- σ_k = Constant in the k- ϵ turbulent model
- σ_ϵ = Constant in the k- ϵ turbulent model
- y_1 = 1) Flow depth on step (cm)
2) Depth in section 1 (cm)
- μ_t = Turbulent viscosity
- ΔH = Dissipated energy in the length of the chute
- a = Variable in the Chamani and Rajaratnam Equation
- b = Variable in the Chamani and Rajaratnam Equation
- g = Gravitational acceleration (m/s^2)
- h = Step height (cm)
- k = Turbulence kinetic energy
- l = Step length (cm, m)
- L = Length in dimension analysis (m)
- M = Mass in dimension analysis (kg)
- m = 1) Height of slope + end sill (mm)
2) Basic variables (Pi Buckingham Theorem)
- n = Number of variables in the Pi Buckingham Theorem

N = Number of steps
 P = End sill height (mm)
 q = Unit discharge ($m^3/m \cdot s$)
 r = Basic (main) parameters in dimension analysis
 S = Chute slope
 T = Time in dimension analysis (second)
 t = 1) End sill thickness (mm)
2) time (s)
 w = Height caused by the slope in inclined step (mm)
 x = Direction
 Z = Distance to the baseline (m)
 k = All parameters in dimension analysis
 α = Energy loss coefficient
 ε = Turbulence energy dissipation rate
 μ = Dynamic viscosity (kg.m/s)
 π = Pi In Buckingham Method

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An Investigation on the Effect of Rail Corrugation on Track Response

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Abstract: Rail corrugation increases life cycle cost of both track and vehicle and is one of the main reasons of track and vehicle defects. To address this problem, this paper explores the effect of rail corrugation on track response. A Finite Element model developed to consider vehicle and track characteristics. Vehicle is a 10 degree of freedom mass-spring-dashpot model which can simulate vertical displacements and rotations. Rail is modeled as an Euler-Bernoulli beam with two degrees of freedom at each node which lies on discrete support to simulate sleeper and fastening system support. The total train-track matrices of mass, damping and stiffness have been formed. Solving the differential equations of motion in time domain for each time step results the response of track to train dynamic forces. A sensitivity analysis has been performed to explore the effect of different train and track parameters on rail displacement. The results of analyses show the effect of corrugation depth and wavelength as well as train speed and axle load on rail deflections and demonstrate the importance of each parameter in the studied range.

Keywords: Vehicle, track, corrugation, rail displacement, train speed

1. INTRODUCTION

Corrugation is major source of dynamic forces applied from vehicles. Based on AREMA (American Railway Engineering Maintenance of way Association), Corrugation initiates from rail head de-carbonization and irregularities such as; rail manufacture pitting, contact fatigue defects, rail welds, rail joints, etc. [1] Train axle load and speed are also important factors creating corrugation with specific wavelengths. Corrugation can be characterized by its depth and wavelength. Different depth and frequency can be detected in the field. UIC (International Union of Railways) divided corrugation into two categories: short-pitch corrugation with wavelength between 3 to 8 cm and long-pitch corrugation with wave length between 8 to 30 cm [2].

The importance of corrugation made many researchers to study this phenomenon to investigate causes, characteristics and treatment of corrugation. These studies, delved into different aspects of rail corrugation both theoretically and experimentally to consider the effect of different track types, vehicle condition, curvature and wheel-rail interaction [3].

Grassie reviewed different type of corrugation and proposed treatments. The effect of vehicle, rail type and traffic were also investigated[4].

Hempelmann and Knothe using an advanced linear model and based on assuming a feedback between structural dynamics and wear explained the formation of short pitch corrugation [5].

Egana et al conducted a research to study the influence of rail pad stiffness on rail corrugation. They concluded that soft rail pads can decrease the growth of corrugation and also eliminate one of the wavelengths [6].

Correa et al taking into account the dynamics of the track, the wheelset and the wear mechanism, developed a numerical method and investigated the effect of track radius on

corrugation for four types of ballasted and ballastless high speed tracks [7].

Although the above mentioned papers and some other researches successfully addressed some important aspects of rail corrugation, the great influence of this rail flaw on deteriorating track and damaging wheels makes more research necessary. The aim of this paper is to investigate the effect of different parameters of corrugation and train on rail displacement using a numerical solution. The numerical method includes modeling of vehicle and track in time domain. The investigated parameters are, corrugation depth and wavelength, train speed and axle load. The purpose is to find the maximum response of track to each parameters in order to control the effective factors on corrugation and prioritize the maintenance activities. The results of the study can be used from freight to high-speed trains.

2. MODELING PROCEDURE

Although it is shown that the combination of physical and numerical modeling provide better results compared to numerical analysis in engineering application, [8], [9], [10] however numerical modeling considering realistic values may lead to good results. This is especially valid for a complicated problem of rail dynamic analysis. In this research a finite element model has been developed to consider the effect of rail corrugation on track response. The model consists of vehicle, track and their interactions. As 0 shows, the vehicle is a ten degree of freedom (DOF) mass spring damper model including a car body, two bogie frames and four wheel-sets. The car body has a mass of M_c and a rotational moment of j_c about the transverse horizontal axis. Bogies have mass of m_t and rotational moment of j_t . Wheels are characterized by a mass of m_w and have one DOF. It is assumed that the mass of each part is concentrated in the centroid of the tack components. the mass, stiffness and damping matrices of train can be expressed as follows: [11], [12]

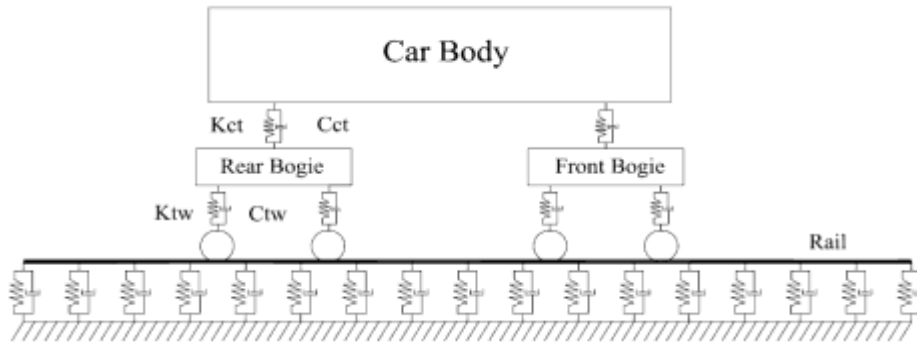


Figure.1 Vehicle and track model

$$[M]_v = \text{diag}[m_c \quad j_c \quad m_t \quad j_t \quad m_t \quad j_t \quad m_{w1} \quad m_{w2} \quad m_{w3} \quad m_{w4}] \quad (1)$$

$$[K]_v = \begin{bmatrix} 2k_t & 0 & -k_t & 0 & -k_t & 0 & 0 & 0 & 0 & 0 \\ 0 & 2k_t L_c^2 & -k_t L_c & 0 & -k_t L_c & 0 & 0 & 0 & 0 & 0 \\ -k_t & -k_t L_c & k_t + 2k_w & 0 & 0 & 0 & -k_w & -k_w & 0 & 0 \\ 0 & 0 & 0 & 2k_w L_t^2 & 0 & 0 & -k_w L_t & -k_w L_t & 0 & 0 \\ -k_t & -k_t L_c & 0 & 0 & k_t + 2k_w & 0 & 0 & 0 & -k_w & -k_w \\ 0 & 0 & 0 & 0 & 0 & 2k_w L_t^2 & 0 & 0 & -k_w L_t & -k_w L_t \\ 0 & 0 & -k_w & -k_w L_t & 0 & 0 & k_w & 0 & 0 & 0 \\ 0 & 0 & -k_w & -k_w L_t & 0 & 0 & 0 & k_w & 0 & 0 \\ 0 & 0 & 0 & 0 & -k_w & -k_w L_t & 0 & 0 & k_w & 0 \\ 0 & 0 & 0 & 0 & -k_w & -k_w L_t & 0 & 0 & 0 & k_w \end{bmatrix} \quad (2)$$

$$[C]_v = \begin{bmatrix} 2c_t & 0 & -c_t & 0 & -c_t & 0 & 0 & 0 & 0 & 0 \\ 0 & 2c_t L_c^2 & -c_t L_c & 0 & -c_t L_c & 0 & 0 & 0 & 0 & 0 \\ -c_t & -c_t L_c & c_t + 2c_w & 0 & 0 & 0 & -c_w & -c_w & 0 & 0 \\ 0 & 0 & 0 & 2c_w L_t^2 & 0 & 0 & -c_w L_t & -c_w L_t & 0 & 0 \\ -c_t & -c_t L_c & 0 & 0 & c_t + 2c_w & 0 & 0 & 0 & -c_w & -c_w \\ 0 & 0 & 0 & 0 & 0 & 2c_w L_t^2 & 0 & 0 & -c_w L_t & -c_w L_t \\ 0 & 0 & -c_w & -c_w L_t & 0 & 0 & c_w & 0 & 0 & 0 \\ 0 & 0 & -c_w & -c_w L_t & 0 & 0 & 0 & c_w & 0 & 0 \\ 0 & 0 & 0 & 0 & -c_w & -c_w L_t & 0 & 0 & c_w & 0 \\ 0 & 0 & 0 & 0 & -c_w & -c_w L_t & 0 & 0 & 0 & c_w \end{bmatrix} \quad (3)$$

In equations (1) to (3), L_c is half of the distance between two bogies and L_t is the half of the distance between two wheels of the same bogie. K_t , K_{tw} , C_t and C_{tw} denote stiffness and damping of the secondary and primary suspension system of the vehicle respectively. K_w and C_w are the spring and damping constants between the rail and vehicle. 0 show the parameters and the assigned values in numerical analysis.

Table 1. Rail vehicle properties

Parameter	Value
Mass of car body (kg)	49500
Car body inertia moment(kg.m ²)	2.15×10 ⁶
Mass of bogie (kg)	3200
bogie inertia moment(kg.m ²)	4000
Distance between bogie centers (m)	12.5
Mass of wheel axle (kg)	900
Secondary suspension stiffness (N/m)	1.74×10 ⁵
Secondary suspension damping (N.s/m)	4.50×10 ⁴
Primary suspension stiffness (N/m)	6.33×10 ⁵
Primary suspension damping (N.s/m)	4.08×10 ⁴

The track and its supporting layer were modeled as beam and discrete mass-less springs and viscous dampers. The springs represent the track sub-layers, connecting the beam to the subgrade. Neglecting axial deformations, each beam element has four DOF which can be described by Cubic Hermitian shape functions. Therefore, displacements of the beam elements'

nodes can be calculated by the following expression. [12], [13]

$$y(e, t) = N(e) \times q_i(t) \quad (4)$$

Where $y(e, t)$ is the vertical displacement of the rail element. $q_i(t)$ is the nodal displacement vector of rail and $N(e)$ is the matrix of the beam shape functions as follows:

$$N_1(e) = [N_1(e) \quad N_2(e) \quad N_3(e) \quad N_4(e)] \quad (5)$$

Where

$$N_1(e) = 1 - \left(\frac{e}{l}\right)^2 + 2\left(\frac{e}{l}\right)^3$$

$$N_2(e) = e \left[1 - 2\left(\frac{e}{l}\right) + 2\left(\frac{e}{l}\right)^2 \right]$$

$$N_3(e) = 3\left(\frac{e}{l}\right)^2 - 2\left(\frac{e}{l}\right)^3$$

$$N_4(e) = e \left[\left(\frac{e}{l}\right)^2 - \left(\frac{e}{l}\right) \right]$$

In which "l" and "e" respectively demonstrate the length and local coordinate of the elements measured from the left node of elements. The mass and stiffness matrices of beam elements (M_r and K_r) can be written in the following form:

$$[M_r] = \frac{\bar{m}l}{420} \begin{bmatrix} 156 & 22l & 54 & -13l \\ 22l & 4l^2 & 13l & -3l^2 \\ 54 & 13l & 156 & -22l \\ -13l & -3l^2 & -22l & 4l^2 \end{bmatrix} \quad (6)$$

$$[K_r] = \frac{E_r I_r}{l^3} \begin{bmatrix} 12 & 6l & -12 & 6l \\ 6l & 4l^2 & -6l & 2l^2 \\ -12 & -6l & 12 & -6l \\ 6l & 2l^2 & -6l & 4l^2 \end{bmatrix} \quad (7)$$

Where \bar{m} , E_r and I_r stand for the mass per unit length, the modulus of elasticity and the moment of inertia of beam elements, respectively.

Considering the mass, stiffness and damping matrices of the vehicle and track elements, the dynamic equation of the whole system can be presented in the following format.

$$[M]\{\ddot{y}\} + [C]\{\dot{y}\} + [K]\{y\} = \{P(t)\} \quad (8)$$

Where, [M], [C], and [K] are the matrices representing mass, damping and the stiffness of train-track coupling system, respectively. $\{y\}$, $\{\dot{y}\}$ and $\{\ddot{y}\}$ are displacement, velocity and acceleration of train-track elements, respectively. P(t) indicates the vector of load induced by the passage of the train. Table. 2 shows track parameters used in numerical analysis. Note that the length of beam elements is assumed to be 0.6 m which is the typical distance between cross ties. So the model has 80 elements and 81 nodes and consequently, the total number of DOFs for rail is 162.

Table 2. Rail track properties

Parameter	Value
Track length (m)	48
Rail modulus of elasticity (N/m ²)	2×10^{11}
Rail moment of inertia (m ⁴)	2.34×10^{-5}
Mass per unit length of rail (Kg/m)	55
Distance between sleepers (m)	0.6

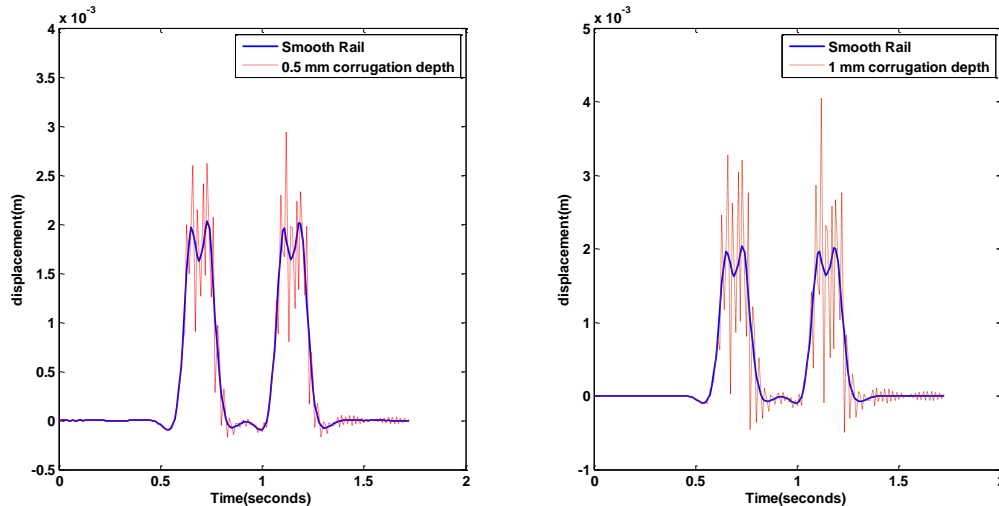


Figure. 2 Rail displacement for different rail corrugation depth (left) 0.5 mm (right) 1 mm

3. VEHICLE-TRACK SYSTEM

Hertz contact theory is used to model the interaction between vehicle and track structure. Neglecting rail irregularities, the contact force between wheel and rail may be determined using Hertz theory through the following formula:[14]

$$P = K_H (y_{wheel} - y_{rail}) \quad (9)$$

Where K_H is linearized Hertzian spring constant which is a function of wheel and rail profile radius and their material properties.

To solve the dynamic equations of motion, Newmark integration method is used. This method developed by Newmark (1959) is based on the assumption that the acceleration varies linearly between two instants of time. The following formula can be applied

$$\dot{u}_{i+1} = \dot{u}_i + [(1 - \gamma)\Delta t] \ddot{u}_i + (\gamma\Delta t) \ddot{u}_{i+1} \quad (10)$$

$$u_{i+1} = u_i + \dot{u}_i \Delta t + [(0.5 - \beta)(\Delta t)^2] \ddot{u}_i + [\beta(\Delta t)^2] \ddot{u}_{i+1} \quad (11)$$

Where Δt is time step, γ and β show the variation of acceleration during one time step. In the numerical solution, the values of γ and β are 0.5 and 0.25, as a result, the solution will be unconditionally stable. Time step, Δt is chosen 0.005 seconds. Applying equations 11 and 12, the track response at time “t+dt” can be determined if response is known at time “t”. [13]

4. RESULTS

Error! Reference source not found. compares the result of analyses for a smooth track and corrugated track with different depth. The figure shows the rail displacement for 0.5 mm and 1 mm corrugation depth. The maximum displacement in perfect condition is 2 mm. 0.5 mm deep corrugation

increases the rail deflection to 3 mm. **Error! Reference source not found.** depicts the same results for 1mm corrugation. As expected, rail displacement increases with increasing the depth of corrugation and the maximum difference between ideal and defected track displacement is about 100%.

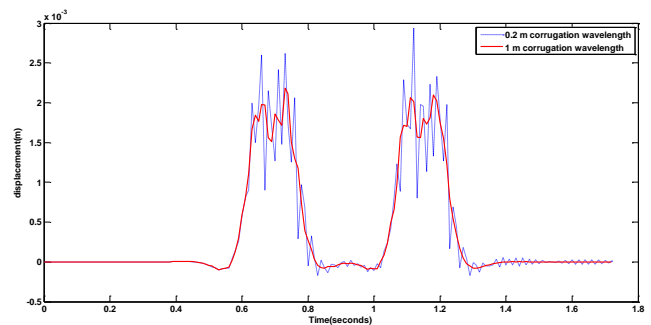


Figure. 3 The effect of corrugation wavelength on rail displacements

To investigate the impact of wavelength on rail response, the analyses are performed for wavelength of 0.2 m and 1 m. 0 demonstrates the effect of corrugation wavelength on rail deflection. Increasing corrugation wavelength causes a reduction in rail displacement. As the figure shows about 40% drop in rail displacement can be seen by increasing the wavelength.

Train axle load is an important parameter to raise rail displacement. This can be seen in 0 which shows the influence of train axle load on rail displacements. It should be noted that to obtain this graph, it is assumed that vehicle speed is 100 km/hr. and wavelength and depth of corrugation are 0.2 m and 0.5 mm. The minimum displacement from the cases

shown in 0 is 2.4 mm corresponding to 10 ton axle load. By increasing the train load, rail displacement increases and for

22 ton axle load reaches to 3.97 mm.

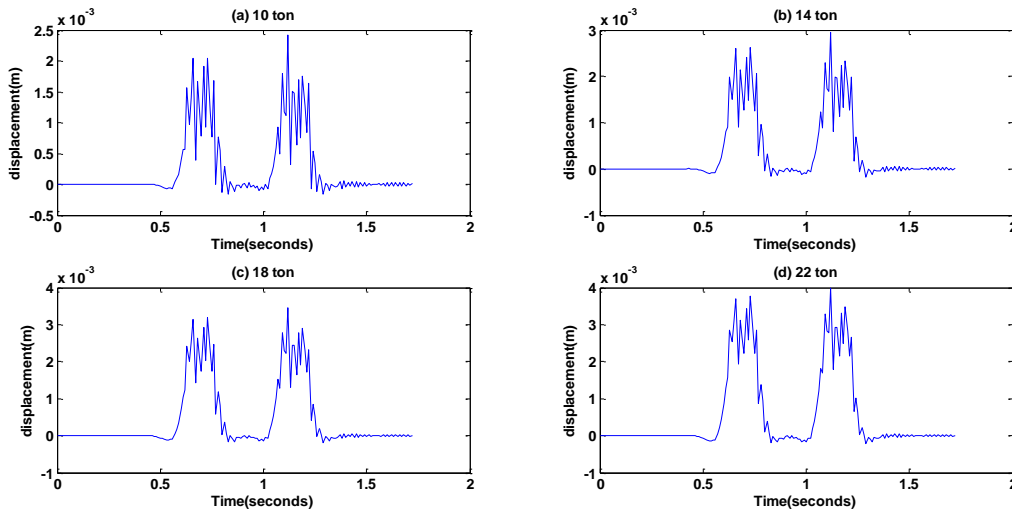


Figure. 4 The effect of axle load on rail displacement

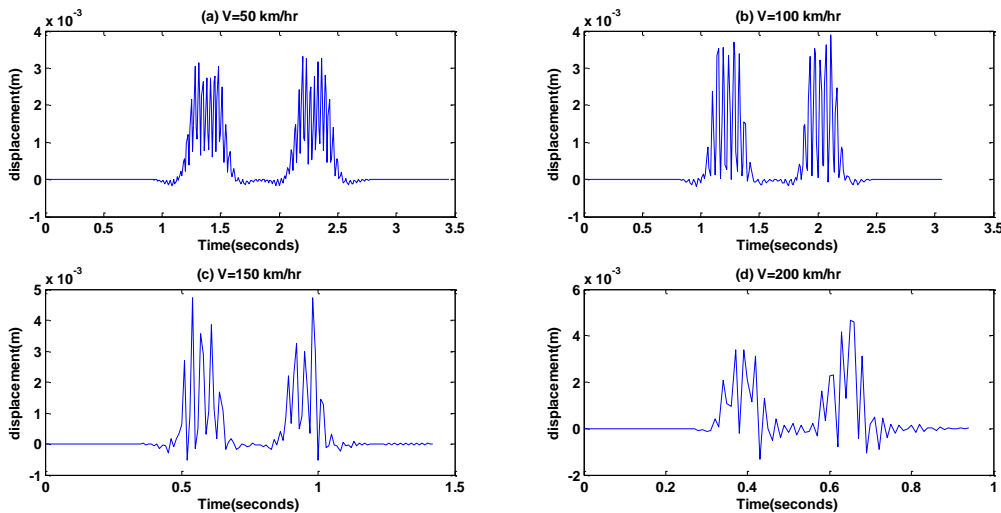


Figure. 5 The effect of train speed on rail displacements

In intercity lines, vehicles with different speeds may travel and the passage of trains with different speeds can create corrugation with varying depth and wavelength. As a result, train speed is one of the most influential parameters on rail response. In this part, it is assumed that axle load is 14 ton and corrugation parameters i.e. wavelength and depth are 0.2 m and 0.5 mm and constants. The results presented for speeds 50, 100, 150 and 200 km/hr.

As 0 shows, the maximum rail displacement under loads moving at the speed of 50 km/hr is 3.1 mm. With increasing vehicle speed, rail displacement also increases and for speed 100 km/hr reaches 3.8 mm. This trend is valid for 150 km/hr. train speed and the maximum deflection raises to 4.7 and. Increasing the speed of vehicle more than this point results in a decrease in rail displacement. The maximum displacement for 200 km/hr train speed is 4.6. As a result, 150 km/hr is the critical speed for this case. 0 illustrates the difference in critical speed with varying corrugation wavelength. An increase in corrugation wavelength results in increasing

critical speed. So in case of high-speed train, long wavelength corrugation should be avoided.

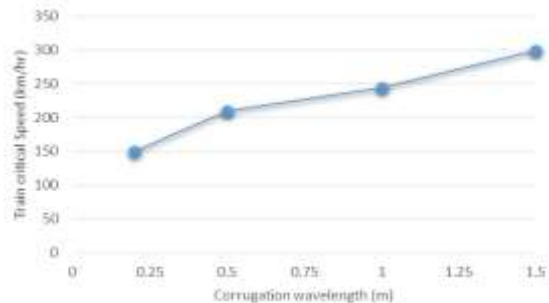


Figure. 6 The effect of corrugation wavelength on train critical speed

5. CONCLUSIONS

This paper explored the influence of corrugation on track displacement by using a finite element model of track and

vehicle. Vehicle is simulated by mass-spring-damper model and rail is considered as Euler-Bernoulli beam and the whole system has been solved in time-domain by Newmark integration method. The results of the study show rail displacement under different conditions and determine the effect of train and track parameters on rail response. The results of the study can be summarized as follows

- Increasing corrugation depth results in about 40% increase in rail displacement. Wavelength have almost the same effect and changing wavelength causes 50% alternation in rail displacement
- The maximum effects of axle load and train speed in the considered range are 58% and 62% respectively.
- Corrugation is a very important factor in increasing dynamic effect of rail vehicles. This is very crucial in case of low wavelength and deep corrugation. Controlling of corrugation depth and wavelength is very important in case of freight and high-speed trains.
- Increasing train speed does not necessarily increases rail deflection. For each case of corrugation wavelength and depth, vehicle critical speed should be determined and considered for design purposes.

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