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CORRESPONDENCE and COMMUNICATION:

Istanbul Gelisim University Faculty of Engineering and Architecture
Cihangir Mah. Şehit P. Onb. Murat Şengöz Sk. No: 8
34315 Avcilar / Istanbul / TURKEY
Phone: +90 212 4227020 **Ext.** 221
Fax: +90 212 4227401
e-Mail: ijet@gelisim.edu.tr
Web site: http://ijet.gelisim.edu.tr
http://dergipark.ulakbim.gov.tr/ijet
Twitter: @IJETJOURNAL

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Anka Matbaa
Sertifika No: 12328
Tel: +90 212 5659033 - 4800571
e-Posta: ankamatbaa@gmail.com

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Dear Colleagues,

On behalf of the editorial board of International Journal of Engineering Technologies (IJET), I would like to share our happiness to publish the fifth issue of IJET. My special thanks are for members of editorial board, editorial team, referees, authors and other technical staff.

Please find the fifth issue of International Journal of Engineering Technologies at http://dergipark.ulakbim.gov.tr/ijet. We invite you to review the Table of Contents by visiting our web site and review articles and items of interest. IJET will continue to publish high level scientific research papers in the field of Engineering Technologies as an international peer-reviewed scientific and academic journal of Istanbul Gelisim University.

Thanks for your continuing interest in our work,

Professor ILHAMI COLAK
Istanbul Gelisim University
icolak@gelisim.edu.tr

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H_2-Anion Interactions and Energy Calculations for Imidazolium-based Ionic Liquids as Hydrogen Storage Materials

Mustafa Karakaya*‡, Fatih Ucun**

*Department of Energy Systems, Faculty of Engineering & Architecture, Sinop University, Sinop 57000, Turkey

**Department of Physics, Faculty of Arts and Sciences, Süleyman Demirel University, 32260 Isparta, Turkey

(mkarakaya@sinop.edu.tr, fatihucun@sdu.edu.tr)

‡ Corresponding Author; Mustafa Karakaya, Sinop University, Sinop 57000, Turkey, Tel.: +90 368 2715516 Fax: +90 368 2714152, mkarakaya@sinop.edu.tr

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Abstract-The aims of this study are to explore the molecular hydrogen-anion interactions and assess the energy calculations in imidazolium-based compounds. The stable modes were structurally discussed after the achieving optimizations by density functional theory. It is concluded that the interaction energies were very weak against the strong interaction lengths. The impacts of the loaded molecular hydrogen to the imidazolium-based structure were discussed by the frontier molecular orbital analysis. While the amounts of H_2 involved to the interaction increased, the changes in the energy gap were calculated. The bonding interactions on the cation–anion and molecular $n$$H_2$–anion were compared.

Keywords: Hydrogen storage materials, ionic liquids, imidazolium, molecular H_2 interactions.

1. Introduction

Hydrogen, being alternative to conventional energy sources such as natural and fossil fuels in recent years, is an important research topic to prevent global climate change and continuously meet the increasing energy demand [1]. The development of hydrogen fuel cells is also increased the activities on high-capacity hydrogen-containing materials aimed hydrogen storage [2].

Hydrogen storage-based studies have certain disadvantages such as continuous boil-off for liquid hydrogen, low capacity in use of compressed hydrogen gas and lack of safety concerns under high pressures [3]. So, materials-based scientific studies for hydrogen storage have been focused on composite materials, metal hydrides, ammonia borane, amides, metal organic structures and organic liquids [1]. Metal borohydrides with a high hydrogen capacity also has been the subject of many researchers [4-6]. Ammonium borane (AB) and derivatives are also structures comprising the high hydrogen, ~19 wt%, and this value is reduced to ~14 wt% in partial dehydrogenation of AB because of that the full dehydrogenation occurs at higher temperatures than 500 ºC [7]. Ionic liquids (ILs) are eco-friendly solvent widely used in green energy applications to avoid environmental concerns and attract attention with the chemical-electrochemical characteristics in fields such as better thermal stability, lithium batteries and electrochemical capacitors [8-10]. Besides, ILs are more special structures about ionic, covalent interactions, pi-stacking and hydrogen bonding according solvents [11-14].

Newly researches on the role of imidazolium ILs, hydrogen storage materials, for H_2 generation from AB derivatives [15], thermal dehydrogenation of ethylene diamine bisborane [16, 17] and physicochemical properties of the several synthesized imidazolium ILs [3, 18-20] are available. In addition, quantum calculations on imidazolium-derivative ILs are enriched to the literature such as hydrogen bond interactions among the ion pairs [21-23], structural and spectral analysis etc. [24]. We wish to investigate the interaction energy between BF_4^-, PF_6^-, HCO_3^- anions and molecular H_2 for the 1-butyl-3-methylimidazolium structures in this study. 1-butyl-3-methylimidazolium tetrafluoroborate ($[BMIM]^+BF_4^-$), 1-butyl-3-methyl imidazolium hexafluorophosphate ($[BMIM]^+PF_6^-$) and 1-butyl-3-methylimidazolium hydrogen carbonate ($[BMIM]^+HCO_3^-$) structures have been selected. In the first part, the lowest energy conformers have been studied in order to highlight the anions–$n$$H_2$ interactions. Interaction energies, frontier orbitals and spectral data have been calculated and interpreted for the anions subjected to interact with $n$$H_2$ in the next stage.

2. Computational details

In this work, all the quantum calculations on the structural optimizations, theoretical spectral characteristics, interaction energies with $n$$H_2$ and molecular orbitals have been performed using density functional theory (DFT) [25] and Becke's three-parameter exchange function [26] combined with the exchange functional component of Perdew and Wang (B3PW91) [27], 6-31G (d) basis set level. Datta and Pati have reported that the PW91 function provided more successful outcomes than B3LYP related physical adsorption of molecular hydrogen for circulene derivatives [28]. Inputs on the atomic coordinates and the identification of redundant coordinates for all geometry optimizations and potential surface scans, respectively, have been formed by Gauss View software database [29]. All the optimizations on geometries of ion pairs and molecular H_2 interactions have been performed by using Gaussian 09W program package [30]. Basis set superposition error (BSSE) corrections and interaction energies between fluorides with molecular H_2 have been calculated by the counterpoise correction procedure (CP) [31]. The partial densities of states (PDOS) spectral analysis for each of the groups of atoms and contributions of the molecular orbitals have been performed by the agency of GaussSum Version 3.0 [32].

3. Results and discussion

3.1. Structural investigations on interactions

Firstly, we focused on exploring of the most stable conformation for $n$$H_2$ interactions. Taking into account molecular H_2 interactions, it is obvious that the clustering dihydrogen structures around anions (BF_4^-, PF_6^- and HCO_3^-) have minimum energies due to the strong electronegative effects. An imidazolium-based structure involving the interaction with +4H_2 is shown in Fig.1.

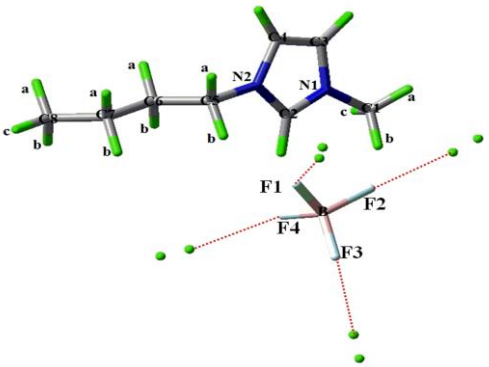

Fig. 1. Optimized structure of [BMIM]BF_4 that emphasizes the interaction between BF_4^- and molecular H_2

Total SCF energy, relative energy, structural properties of a single H_2 interaction and the impacts on [BMIM]$^+BF_4^-$ such as fluorine-dihydrogen distance are interpreted in the first section. For the single H_2 interaction, the most stable conformations have been determined in F1···H_2 interaction and, total energy value for the whole structure, [BMIM]BF_4···H_2, is equal –848.68806 a.u. in quantum chemistry calculations. In other single H_2 interactions, F2···H_2, F3···H_2 and F4···H_2, relative energies of [BMIM]BF_4···H_2 are at very small values of 0.09, 0.30 and 3.37 kJ/mol, respectively. F1···H_2 distance is approximately 2.449 Å and others are increased in the range of 2.449–2.480 Å.

The graphic obtained by data of optimized potential surface scan is given as Fig. 2. Potential energy surface (PES) computation is performed to determine the position of H_2 molecule in stability of the BF_4–H_2 interaction. Total energies of [BMIM]BF_4···H_2 structure are obtained by 0.125 Å increments of the each interaction distance from 2.000 Å to 3.125 Å in total step numbers of 10. Scan coordinates selected as F1–H_2 interaction distances are variables of the x-axis and y-axis represents relative energies, ΔE, to the total energy of [BMIM]BF_4···H_2 structure (F1–H_2 interaction) in Fig. 2. Minimal relative energies are in the range of 2.375–2.500 Å. These results support the optimizations in the conformation analysis regarding molecular H_2 positioning.

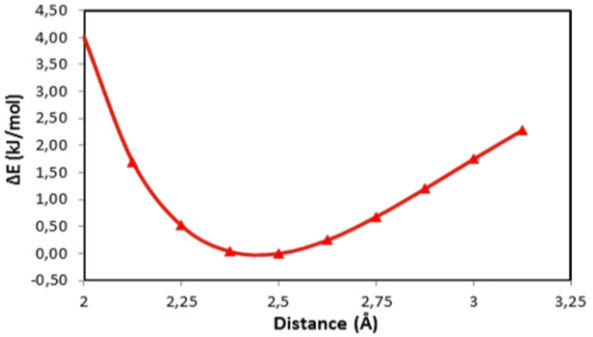

Fig. 2. Variation graph of relative energy with to F1–H_2 interaction distances for [BMIM]BF_4···$n$$H_2$ structure

Fig. 3 shows the variations of BSSE corrected and uncorrected binding energies by the F1···H_2 distances in single molecular H_2 interaction. Even though uncorrected binding energy between fluorine (F1) and H_2 is the minimal value in ~2.500 Å, minimal interaction energy is in ~3.125 Å in BSSE corrected calculation. While the anion-H_2 distances increase, interaction energies are closer to zero in both calculations (BSSE corrected and uncorrected). Also, it is remarkable that the BSSE corrected binding energy passes through negative value in 2.500–2.625Å.

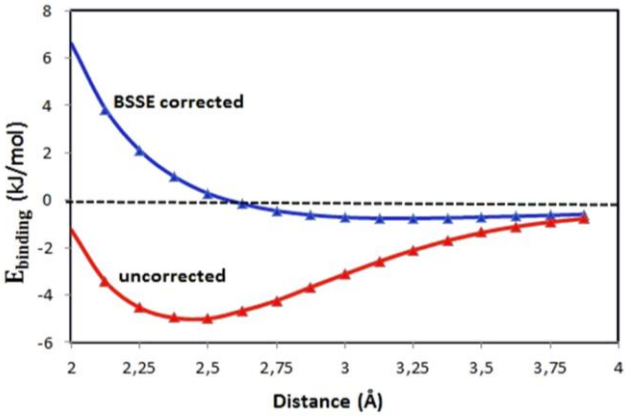

Fig. 3. BSSE corrected and uncorrected interaction energies of the molecular H_2 (single) corresponds to F1–H_2 interaction distances

Total energies and interaction energies in the anion–H_2 interactions for the various imidazolium-based structures have been listed in Table 1. While the numbers of hydrogen molecules included to anion interactions increases, the average interaction energies per H_2 mostly decreases in uncorrected and BSSE corrected calculations. For the zero point energy (ZPE) corrected calculations, the interaction per H_2 is stronger except for the PF_6–H_2 interaction, while the amount of H_2 increases. In a previous study, the averaged adsorption energies (ZPE corrected) between a lithium functionalized naphthalene and $+3H_2$, $+6H_2$ are calculated as 0.04, 0.02 eV (respectively), and these results are evaluated as the weak interactions with H_2 molecule [33]. Also, the fluorine–hydrogen distances (average values) for BF_4, PF_6 and oxygen–hydrogen distances for HCO_3 anion have been listed in Table 1. The average lengths have been calculated within the range 2.449–2.538 Å from the added single H_2 up to $8H_2$ for the [BMIM]BF_4···nH_2 complex. Similarly, structural parameters have resulted as 2.618, 2.656 Å and 2.432, 2.524 Å in [BMIM]PF_6···nH_2 and [BMIM]HCO_3···nH_2, respectively. While the amounts of H_2 molecules added to the system increased, the binding abilities have decreased for all investigated compounds. The BSSE corrected interaction energies per H_2 have decreased and, anion–H_2 distances have increased depending on the increase in the amount of H_2 molecules for [BMIM]BF_4···nH_2 and [BMIM]HCO_3···nH_2 complexes. The calculations on the uncorrected interaction energies per H_2 contain these results for all complexes. Binding energies of up to loading 10 H_2 molecules to octathio[8]circulene are within the range –0.70 kcal/mol ($+H_2$) and –4.5 kcal/mol ($+10H_2$) and the distance between single H_2 molecule (vertically) and thiophene ring is 3.2 Å [28]. In a study of the H_2 adsorption on pure carbon nanotubes, the calculated binding energy for adsorbed H_2 molecule are ~57 meV and this results are assessed as the weak physical adsorption [34].

In the present work, the uncorrected interaction energies are close to the binding energies for these complexes with physisorption property. However, distances between the H_2 and anions are smaller. The small distance in H_2 interactions makes it difficult to store the hydrogen molecules whereas planar structures providing large surface areas are also effective for molecular hydrogen storage according to Datta and Pati [28]. For reasons highlighted above, despite of reasonable interaction energies, it is thought that the investigated ionic liquids are structurally unfavorable in terms of hydrogen storage.

Table 1. Energy values in the interactions and distances between imidazolium structures with the hydrogen molecules by ab initio calculations

Complex	Total SCF Energy (a.u.)	Interaction energy -uncorrected- (kJ/mol)	Interaction energy -BSSE corrected- (kJ/mol)	Interaction energy -ZPE corrected*- (kJ/mol)	Δd** (Å)
$[BMIM]^+BF_4^-$					
$+H_2$	-848.688	-4.997	0.553	-1.321	2.449
$+2H_2$	-849.864	-9.568 (-4.784)	1.013 (0.507)	-3.067 (-1.534)	2.468
$+4H_2$	-852.216	-18.938 (-4.735)	1.829 (0.457)	-7.506 (-1.877)	2.469
$+8H_2$	-856.919	-35.045 (-4.381)	3.114 (0.389)	-16.289 (-2.036)	2.538
$[BMIM]^+PF_6^-$					
$+H_2$	-1364.714	-2.979	0.227	-1.861	2.618
$+6H_2$	-1370.592	-17.345 (-2.891)	2.164 (0.361)	-10.730 (-1.788)	2.656
$[BMIM]^+HCO_3^-$					
$+H_2$	-688.693	-6.555	-1.581	-0.549	2.432
$+3H_2$	-691.046	-15.352 (-5.117)	-2.138 (1.069)	-4.096 (-1.365)	2.524

* The interaction energy with zero point energy correction.
** d[$F^{\cdots}H_2$] average values are for [BMIM]BF_4 and $[BMIM]^+PF_6^-$.
d[$O^{\cdots}H_2$] average values are for $[BMIM]^+HCO_3^-$.
The values in parentheses are average interaction energies per H_2.

3.2. Molecular orbital analysis

HOMO and LUMO energies as frontier molecular orbitals (FMO's) are important to define the optical, electrical properties of compounds in quantum chemistry calculations, and act as electron donor and acceptor, respectively. [35–37]. The frontier molecular orbitals and energy diagrams of [BMIM]BF_4 and $+nH_2$ have been shown in Fig. 4. The positive and negative wave functions for the molecular orbitals are shown in red and blue tones, respectively. Although the HOMO plot is scattered over the imidazolium moiety in cation and anion, LUMO is over the imidazolium structure, entirely. While the amounts of H2 involved to the interaction increase, HOMO plot on BF_4 anion decreases and the energy gap between the FMO's also increases.

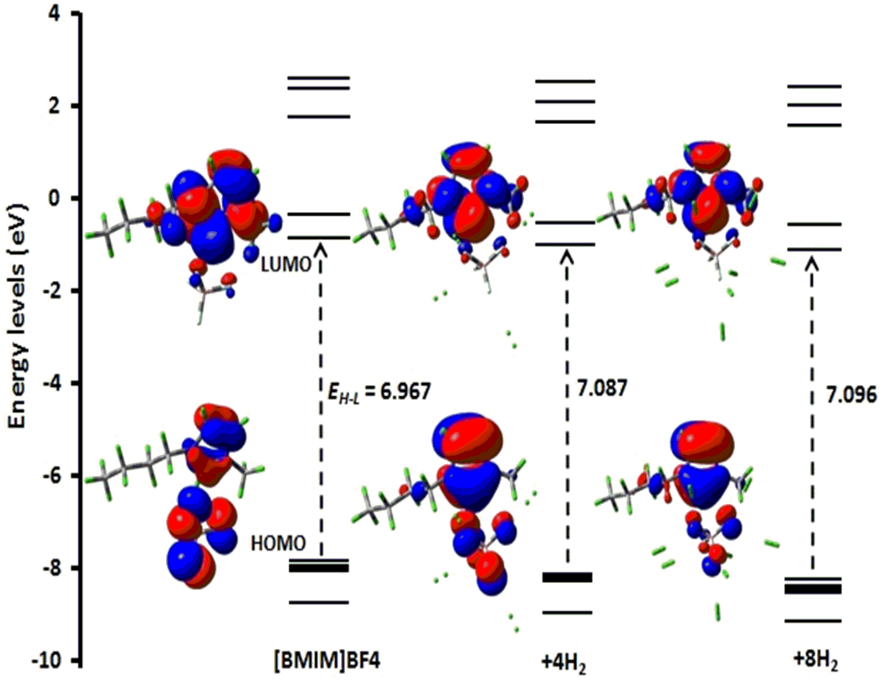

Fig. 4. Molecular orbital energy levels, boundary ranges and HOMO-LUMO visuals for $[BMIM]BF_4\cdots nH_2$ structures

The energy gaps between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) in the selected IL's$\cdots nH_2$ are given in Table 2. While the amounts of H_2 subjected to interaction increases, it is noteworthy that the differences in HOMO-LUMO energy gap are much higher than the BSSE corrected interaction energies. The changes of HOMO-LUMO energy gaps are much less than the adsorption energies, and this result has been interpreted as associated with the H_2 adsorption property of sumanene in a previous study [38]. Also, the HOMO-LUMO energy gaps in complexes (excepting $[BMIM]^+PF_6^-\cdots H_2$) that interact with the hydrogen molecules are higher than the gaps of pure $[BMIM]^+BF_4^-$, $[BMIM]^+PF_6^-$ and $[BMIM]^+HCO_3^-$ structures in this study.

Table 2. Energy gaps of the frontier molecular orbitals obtained by ab initio computing

Complex	ΔE_{H-L}* (kJ/mol)	Relative values in ΔE_{H-L} (kJ/mol)
$[BMIM]^+BF_4^-$	672.192	0.000
$+H_2$	676.070	3.878
$+2H_2$	677.807	5.615
$+4H_2$	683.789	11.597
$+8H_2$	684.658	12.466
$[BMIM]^+PF_6^-$	685.478	0.000
$+H_2$	685.333	-0.145
$+6H_2$	691.508	6.030
$[BMIM]^+HCO_3^-$	447.208	0.00
$+H_2$	453.480	6.272
$+3H_2$	461.005	13.797

* Energy gap between *highest occupied molecular orbital* and *lowest unoccupied molecular orbital* for the complex.

3.3. Spectral properties

The calculated ^1H and ^{13}C NMR chemical shifts (with respect to TMS) for $[BMIM]BF_4$ and the changes in $[BMIM]BF_4\cdots nH_2$ interactions have been listed in Table 3. When the results are compared with the experimental data [8] obtained from the literature, it can be said that the mean absolute errors (MAE) have reasonable values. The carbon and hydrogen atoms in the table are numbered according to the model in Fig. 1.

The chemical shifts in C2 (138.8 ppm), C3 (113.2 ppm), C4 (114.8 ppm) and H2 (10.86 ppm), H3 (6.49 ppm), H4 (6.52 ppm) are higher, compared with the ones of the other carbons. The high chemical shifts can be attributed to its proximity to the nitrogen atoms owner electronegative property. The chemical shift values of carbon and hydrogen atoms in the methyl and methylene groups are also small as expected. The most significant changes in the chemical shifts of $[BMIM]BF_4\cdots nH_2$ are computed for the C5, C6 and H5b, H6b (see Table 3). ^1H chemical shift changes between $[BMIM]BF_4$ and $BMIM]BF_4$–acetonitrile (CH_3CN) interaction have been computed as 0.64 (for H2), 0.44 (H3) and 0.45 ppm (H4) by DFT (B3LYP functional) calculations in a previous study [39]. In this study, the changes ($\Delta\delta'$ and $\Delta\delta''$) in ^1H and ^{13}C chemical shifts for the $BMIM]BF_4\cdots 4H_2$ and $+8H_2$ are associated that the electron-withdrawing groups (the attaching of the H_2 molecules) can decrease the shielding [40].

Table 3. Chemical shift values of $[BMIM]BF_4$ and the changes of $[BMIM]BF_4 \cdots n H_2$ interactions in parts per million (ppm) relative to tetramethylsilane by ab initio calculations

Atom	Exp.**	$[BMIM]BF_4$	$\Delta\delta'$ (in $[BMIM]BF_4 + 4H_2$)	$\Delta\delta''$ (in $[BMIM]BF_4 + 8H_2$)
C1	36.04	35.08	0.209	0.251
C2	135.99	138.82	0.167	0.732
C3	123.80	113.23	1.398	1.845
C4	126.50	114.83	0.474	0.364
C5	49.57	52.21	2.135	2.126
C6	31.86	30.53	4.886	4.894
C7	19.25	22.28	0.179	0.237
C8	13.27	15.54	0.003	0.020
	MAE=	*4.413*		
H1_a	3.962	3.173	0.035	0.078
H1_b		5.247	0.013	0.075
H1_c		3.277	0.063	0.113
H2	8.857	10.860	0.001	0.162
H3	7.417	6.490	0.068	0.108
H4	7.257	6.524	0.081	0.120
H5_a	4.191	3.248	0.158	0.225
H5_b		4.662	0.614	0.524
H6_a	1.864	1.422	0.204	0.217
H6_b		3.272	1.437	1.435
H7_a	1.358	1.242	0.136	0.149
H7_b		1.698	0.041	0.052
H8_a	0.959	0.898	0.012	0.006
H8_b		1.298	0.250	0.252
H8_c		1.183	0.083	0.095
$+H_2$*		5.070, 3.864		
	MAE=	*0.752*		

* Chemical shift value in $[BMIM]BF_4+H_2$ and 5.070 ppm is for H close to F1. ** Taken from Ref. [8].

The COOP diagrams are defined as a multiplication of the density of states (DOS) spectrum and the overlap population in the form of positive or negative between two different groups expressed as bonding–antibonding with respect to each of the molecular orbitals [32]. In overlap population analysis, the positive, negative regions and zero line represent the bonding, anti-bonding and nonbonding interactions, respectively [41, 42]. The overlap between BF_4 anion with [BMIM] cation is more intense than ones of BF_4 anion with $+8H_2$ as illustrated in Fig. 5. The bonding interactions on $BF_4^- \cdots 8H_2$ are effective, but weaker than $BF_4^- \cdots [BMIM]^+$ bonding interactions. The interaction energies between anion–cation have been computed in the range of -345.10 and -300.01 kJ/mol for the different four optimized conformers of $[BMIM]^+ \cdots BF_4^-$ complex in a previous study [43]. These results too higher according to the interactions on $BF_4^- \cdots 8H_2$, and support the remarks obtained by the overlap population analysis. The interaction between [BMIM] cation and $+8H_2$ have been also interpreted as nonbonding interactions. In addition, the anti-bonding interactions remain lower than bonding interactions.

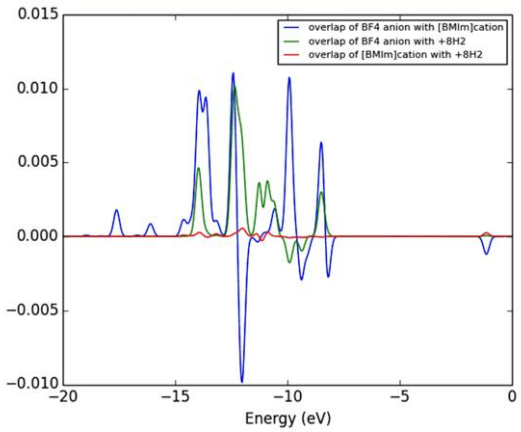

Fig. 5. COOP diagrams between atoms groups in $[BMIM]BF_4 \cdots 8H_2$

4. Conclusions

In this work, a detailed analysis on interactions between the anions of several imidazolium-based compounds and loading molecular hydrogen has been presented with the aid of computational quantum mechanical modelling methods. The BSSE corrected, ZPE corrected and uncorrected interaction energies have been calculated for comparison. It was concluded that the interaction energies are very weak against the strong interaction lengths. It was also seen that the averaged interaction lengths increase while the number of the loading H_2 molecules have increased. The frontier molecular orbitals and energy diagrams are also remarkable on the anion–H_2 interactions. While the amounts of H_2 involved to the interaction increase, the HOMO plots surrounding the anion have decreased, markedly. In the spectral analysis section, the NMR calculations and overlap population diagrams have been reviewed. The significant variation of the chemical shifts in cation have been obtained by NMR calculations and compared with the studies in the literature. We have also found that the bonding interactions on the $BF_4^-\cdots 8H_2$ are effective, but weaker than $BF_4^-\cdots[BMIM]^+$ bonding interactions. Consequently, it is believed that this study will contribute to green energy applications.

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A Comparison Study of Some Flood Estimation Methods in terms of Design of Water Structures

Necati Gulbahar*‡

*Department of Civil Engineering, Faculty of Engineering and Architecture, Istanbul Gelisim University, Istanbul, Turkey.

(ngulbahar@gelisim.edu.tr)

‡Corresponding Author; Necati Gulbahar, Department of Civil Engineering, Faculty of Engineering and Architecture, Istanbul Gelisim University, Istanbul, Turkey, Tel: +90 212 422 7020, Fax: +90 212 422 7401, ngulbahar@gelisim.edu.tr

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Abstract-Flood is a natural disaster that caused the death of many people, environmental destruction and economical loses. Therefore, it is must be taken under control and prevent damage to the people and environment. Particularly, cities and villages have been often faced with floods that result from engineering and planning errors in Turkey. As a conventional approach, some certain calculations methods have been developed in order to estimate flood discharge, velocity, depth and recurrence in this regard. Some of them are widely used for the flood estimation such as; unit hydrograph, stochastic and statistical, Rational, MacMath, Kirpich, Mockus, SCS, Snyder and Degree-Day methods. Because, every method has some significant limiting conditions, each one gives different results for same place. According to recent researches, selection of the proper method is very important to reach more accurate results, but the best one is measuring. Therefore, a suitable method to meteorological, hydrologic, topographic conditions of a basin should be selected for the successful application. In this paper, some common conventional methods were discussed and evaluated for the aim of performing better results.

Keywords: Flood, comparison, structures, rational method

1. Introduction

Throughout the history, humans have wished to settle in the coastal area of river, lakes and sea. Of course, there are many reasons for this attitude. One of the most important reason is that human needs of water for the life and must use it for various purposes in agriculture, industry and other activities. On the other hand, those attractive places are very risky region in terms of natural disasters such as earthquake, flood and, landside. Flood can be defined as it spreads over the land and damages surroundings as water flows at high speed and big discharge. In facts, floods are natural disasters which cause loss of lives after earthquakes in the world.

Generally, in order to design the hydraulic structures, ıt is necessary to obtain the data based on meteorology and hydrology at least 30 years. However, the gauge stations may not be sufficient in terms of quantity and quality in any country.

Looking at the history, the archaeological studies show that floods have damaged to human such as Tigris and Euphrates in Mesopotamia; The Nile in Egypt; Ganges and Indus in India and Yellow River in China.

The first studies in the modern sense began in Netherland in 1544. Recently, European Union (EU) Directive numbered 2000/60/EC with the name of Water Frame Work was emphasized an Integrated Watershed Management and European Parliament and EU Commission with the numbered 2007/60/EC Directive also stated the floods as unavoidable hazard that caused the people's dead, damaged the environment, cultural heritage, economic development and infrastructures. However, it is stated in the same directive that it is also possible to reduce these losses. Therefore, ıt has been made compulsory to do preliminary flood risk assessment, flood hazard maps, flood risk map and flood risk management plans for a member states up to the certain date.

There are some challenges in this regard that need to be fighting in Turkey. According to research of General Management of Natural Disaster, the most common natural disasters are landslide, earthquake and flood have been occurred frequently in the country. From Fig. 1 it can be seen as landslide (45%), earthquake (18%) and flood (14%) frequently occurred in the country. So, this subject is more important for Turkey than Europe.

Another challenge is that, works carried out by institutions are scattered with no cooperation because there is not a general technical regulation covering general rules for combating flood [6].

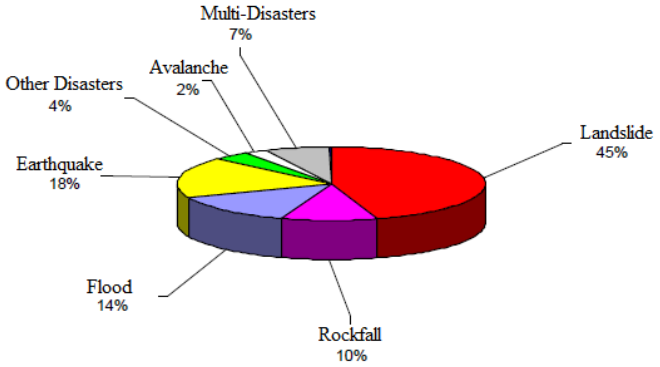

Fig. 1. Distribution of type of disaster [8]

In parallel to works done in Europe, it has been carried out some significant studies in this field under planning and control of General Directorate of State Hydraulics Works (DSI) which is only public authority in flood in Turkey. Besides, it was also stated some necessary measures to be taken at the Directives of Prime Ministry with the numbered 2006/27 Creek Beds and Floods and 2010/5 numbered Rivers and Creek Beds Improvement. However, some important developments have been achieved in this regard recently, such as; creek development, channel capacity enlargement, urban renewal.

Generally, in order to design the structures for flood in any area, the level, magnitude and variation of peak discharge, recurrence of precipitation must be determined. The most common used equations for the estimation of these parameters are known as unit hydrograph, stochastic and statistical method, Rational, Mac Math, Mockus, SCS, Kirpich, Snyder and Degree-Day method.

Since each method has different characteristics and coefficients, different results will be obtained naturally. In this study, these subjects will be discussed and evaluated based on conventional method.

2. Material and Method

Mainly, two approaches have been used for determining flood discharge; one is conventional method the other is simulation by computer. If the necessary hydrological and meteorological data from a gauge stations in a basin can be obtain, then calculation can be made safely. If not available, then synthetic methods can be used for estimation of flood discharge utilizing the values of similar basin.

Another way is that the necessary parameters are determined and scanned by computer which is called simulation method. There are many simulations methods for the subject such as STORM, SWMM, USGS, HEC-RAS and MIKE serious. However, conventional method will be evaluated in this paper.

3. Discussion and Evaluation

Generally, equations of flood discharge were briefly explained and clarified their restrictive conditions at the following.

3.1. Stochastic and statistical method

These methods are based on the extreme distributions of precipitation which are Gumbel, Pearson, log-normal, Gamma that are proposed to use by DSİ in Turkey. However, package programs have been used for using these methods. Probable maximum rainfall depth could be found by the following formula;

$$X = \mu x + K\sigma x \quad (1)$$

Where;

X : maximum precipitation with T year frequency (mm)

μx : arithmetic average of annual rainfall series (mm)

σx : standard deviation of rainfall series (mm)

K : frequency coefficient depending on rainfall series

3.1.1. Unit hydrograph method

The unit hydrograph of a basin is defined as the hydrograph of surface runoff from 1 cm of excess rainfall generated uniformly over the basin at uniform rate during the specific period of time [2]. Accordingly, unit hydrograph of a watershed can be found from falling constant intensity and distributed evenly hydrograph basin Fig. 2. This is a method that results closest to actual values than the other methods. Flow depth is found by measuring the area under the hydrograph;

$$d = V/A = Q*t/A \quad (2)$$

Where;

d: the depth of flow (m)

V: volume of water

Q: discharge

A: area

t: time

There are also some restrictive conditions in the unit hydrograph method. Each basin must have the rainfall and flow data. Usually, this is not possible in practice. In addition, from the precipitation of complex compounds, the separation of individual storm is not easy. Tools may be defective or may not work during rainfall. Under these conditions, the improper results may be obtained. Also, if the basin is very large, the distribution of the precipitation is not uniform throughout the basin. In this case, you need to split basin into smaller sub-basin [11].

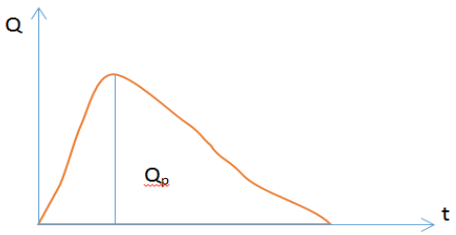

Fig. 2. Unit hydrograph

31.2 Rational Method

It is related rainfall to the corresponding runoff in the basin. It is introduced to scientific community by Kuichling in 1889. This method was developed in USA. It is the simplest and most common used method for flood estimation. The biggest disadvantage of this method is that it cannot be used for large areas. The size of basin should be no more than 25 km2 for this method. Because, total area of basin is considered as least the precipitation should continue until the duration of conservation time. In that case, the probability of precipitation uniformity will decrease. In the other hand, it takes time to fill the surface transmission channels [11].

The idea behind the rational method in that if a rainfall of certain intensity begins instantaneously and continues indefinitely the rate of runoff will decrease until the time concentration. The entire basin continues to flow at the outlet, then stays constant [11]. The formula below shows that, the rainfall intensity is taken equal to the concentration time and C coefficient represents topography and plant cover on the land;

$$Q_p = 0.278*C*I*A \quad (3)$$

$$T_c = 0.0195\ K^{0.77} \quad (4)$$

$$K = L^{3/2} / H^{1/2} \quad (5)$$

Where;

Q_p : the peak flow rate (m^3/s)

C : runoff coefficient (dimensionless)

I : the average rainfall intensity (mm/h)

A : the drainage area (km^2)

L : length of drainage channel (km)

H : the difference between beginning and end of channel

3.1.3. Kirpich's Equation

The equation developed in Tennessee State in USA by Kirpich in 1940 for rural areas where slope in high then 10% and is suitable land cover in timber in more than 59% of area. The formula is preferred because it is simple and easy application [10]. The formulas are given at the following;

$$t_f = t_e/2 + t_p \quad (6)$$

$$t_e = t_r = t_p / 5.5 \quad (7)$$

$$Q_p = k*A*h_a / t_f \quad (8)$$

Where;

Q_p: peak discharge (m^3/s)

t_f : rainfall duration (h)

t_e : effective duration of precipitation

t_p: the time difference between the peak point of hydrograph and the basin center of gravity

h_a : annual rainfall depth for 100 years (cm)

k: coefficient (0.208)

A: area km^2

3.1.4. SCS Equation

In 1957, it is developed for smaller basin than 30 km2 by the U.S. Soil Conservation Service (SCS) in the USA. It has dimensionless triangle hydrograph which is derived from a number of basins in different geographical regions. The advantages and the disadvantages are could be summarized as follows [11];

Advantages:

- It is widely used in basins smaller than 30 km^2
- The equation is simple
- Provides the results close to actual values
- Uses the daily precipitation values

Disadvantages;

- Drainage area should have a curve number
- Drainage area must be homogenous

The equations are given below:

$$t_c = 0.066\ (L^2{}_h / H)^{0.385} \quad (9)$$

$$D = 0.133 * t_c \quad (10)$$

$$L = 0.6 * t_c \quad (11)$$

$$t_p = (D / 2) + L \quad (12)$$

$$S = (1.000 / CN) – 10 \quad (13)$$

$$h_e = (h_a – l)2 / (h_a – l + S) \quad (14)$$

$$Q_p = (0.2083 * A / t_p) * h_e \quad (15)$$

Where;

Q_p : the peak flow rate (m^3/s)

t_p : time of peak (h)

t_f : time of fall (h)

t_c : time of concentration(h)

h_e : maximum flow height (mm)

A : drainage area (km^2)

3.1.5. Mac Math Equation

This method can be used at every type of smooth and undulating land. It gives good results in the calculation of the capacity of surface drainage canals. It does not give good results for the land with steep slopes. The formula is as follows [5] and [11];

$$Q_p = 0.0023*C*I*S^{1/5}*A^{4/5} \quad (16)$$

$$t_c = 0.0195(L^3/H)^{0.385} \quad (17)$$

Where;

Q_p : the peak flow rate (m^3/s)

C : this is a coefficient depending on topography, plant cover and soil

I : Average rainfall intensity for certain recurrence duration and time of concentration (mm/h)

S : slope of the main channel (1000)

A : basin area (ha)

t_c : time of concentration (min)

L : length of basin or channel (km)

H : the difference between beginning and end of channel (m)

3.1.6. Mockus Method

The method which was developed by Victor Mockus is easy to practice and to draw triangular hydrograph. In general triangular hydrographs are sensitive as other normal hydrographs. But, there are some restrictive conditions such as time of concentration up to 30 minutes in the basin, when the recession curve is necessary and selection unit time of rainfall[11].The formulas are as follows;

$$t_c = 0.00032(L_h^{0,77} / S^{0.385}) \quad (18)$$

$$D = 2*t_c^{1/2} \quad (19)$$

$$\Delta D = t_c / S \quad (20)$$

$$t_p = 0.5*\Delta D+0.6*t_c \quad (21)$$

$$q_p = K*A / t_p \quad (22)$$

$$Q_p = q_p*h_a \quad (23)$$

Where;

t_c= time of concentration(h)

L_h= the length of drainage area (m)

S= average slope of drainage area (%)

D= time of duration of precipitation (h)

ΔD= time of heavy rainfall (h)

t_p= the time of duration for peak discharge (h)

h_a= annual rainfall depth of 100 years (cm)

k= coefficient of basin (0.21-1.60)

q_p= discharge generated by 1 mm rainfall

Q_p= discharge generated by 100 years rainfall (m3/s)

3.1.7. Snyder Method

This is one of the synthetic methods to obtain unit hydrograph which was suggested by Snyder in USA in 1938. The main idea of this method is that the basin characteristics which are area, shape, topography, channel slope, stream density are affected the shape of unit hydrograph. After having studied on many hydrographs of the basins in North America, it was defined as a standard unit hydrograph. Snyder method cannot widely used in Turkey, because, basin coefficients are not determined in all basins in Turkey [9,11].

The formulas are given as follows;

$$t_r=t_p/5,5 \quad (24)$$

$$t_p=0,75.C_t\,(L.L_c)^{0,3} \quad (25)$$

$$q_p=2,75.C_p / t_p \text{ peak discharge} \quad (26)$$

$$t_p=t_{pR}+0.25(t_r-t_R) \quad (27)$$

Where;

t_r : effective precipitation

t_p : basin delay (h)

q_p : peak discharge per unit area ($m^3/sec/km^2$)

C_p : basin coefficient

C_t: basin coefficient

There are also some limitations with this formula. If $t_{PR}=5,5.t_R$ then, $t_R= t_r$ and $q_{PR}= q_p$ can be taken, and C_t and C_p can be obtained above equation. C_t and C_p is a function of basin characteristics and slope. If t_{PR} is different from $5,5.t_r$, then basin lag calculated with the following formula;

$$t_p = t_{PR} + 0.25(t_r - t_R) \quad (28)$$

3.1.8. Degree - Day method

Usually, floods from snow melt may occur in any day in the springs. There are some methods for calculation the snow melts. In order to calculate flood from snow melt Degree Day method or some empirical equations could be applied. The degree day method is simple and easy to apply. The basis of the method is that water depth coming from snow melt in a day is proportional with the temperature [2]. The formula is as follows;

$$M=k*T; \quad (29)$$

Where;

M= water level after snowmelt for a day (mm)

K= coefficient of degree day (2-4)

T= temperature (C^o)

As seen above each method has different characteristics. In this regard, recent studies are examined; significant differences can be seen from each other for the same area. Certainly, this is an expected result. In a study conducted for Istanbul, the obtained results are different each other. Table 1 and Table 2 show that Snyder gives maximum values while SCS gives the minimum ones. As a function of topography, maximum value was obtained in Sazlıdere. But, all methods gave close results for only Sariyer.

Table 1. The data of some selected streams [10]

Stream Name	Slope	Area (km^2)	Rainfall Depth (mm)
Alibeykoy	0,0025	34,465	105,00
Ayamama	0,0049	47,903	23,03
Sariyer	0,0095	7,266	24,00
Nakkas	0,00005	44,906	44,29
Kurbagalidere	0,0049	47,304	24,00
Sazlidere	0,00031	52,775	347,14
Tugay	0,0098	24,255	62,22
Kemikli	0,0049	63,020	28,00

Table 2. Comparison of flood discharge for each method [10]

Stream Name	Flood Discharge for 100 years (m^3/s)			
	Snyder	Kirpich	Mockus	S.C.S
Alibeykoy	399,00	262,54	218,16	169,36
Ayamama	122,09	81,66	51,14	44,13
Sariyer	33,60	29,43	35,95	38,92
Nakkas	168,30	117,35	37,75	6,58
Kurbagalidere	117,60	82,68	41,41	36,89
Sazlidere	2291,00	1589,00	124,27	383,83
Tugay	180,53	125,72	109,08	108,26
Kemikli	196,00	135,53	46,20	39,43

According to another study carried out for the same place in Istanbul; Snyder, Mockus, Iszkowski and Lauterburg methods were tested and the results were seen in Fig. 3. The results are completely different from each other. In Fig. 4 Calculated results are compared with reference to measurement results. The results are close to each other for Nakkas and Kurbagalidere, but they are far from each other for Kagithane.

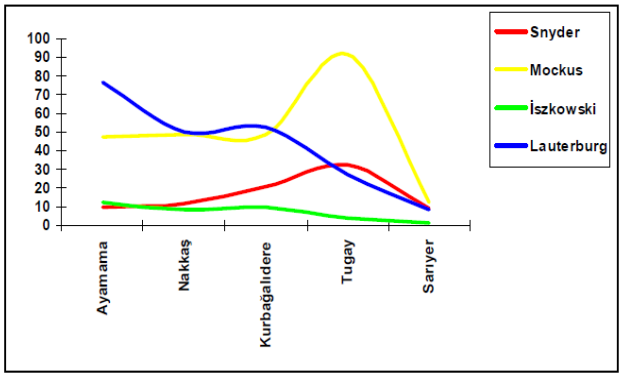

Fig. 3. Comparison of Discharge Values [3]

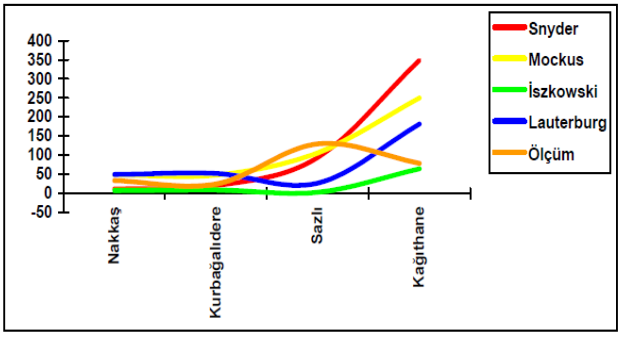

Fig. 4. Comparison of methods used and measurement [3]

4. Conclusion

Generally, differences observed from equations are resulted from both basin and equations. Considering basin, each basin has different meteorological, topographical, hydrologic, hydraulic conditions. Each basin may have not gauge station. On the other hand, assumptions of the equations and coefficient are different each other. All methods are based on a uniform distribution of precipitation in a given area which is not possible in nature.

Hydrological events have variable and uncertainty characteristics. Therefore, they contain both deterministic and stochastic components. In these methods, past data have evaluated and estimated future values. Certainly, they also contain some risks.

Because of based on measuring data, the unit hydrograph method results are closest to actual values. Coefficients are not used and assumptions are close to actual situations. If there is no sufficient data, the synthetic hydrograph methods should be used. In that case, similarity should be provided precisely.

One of the common used synthetic methods is Snyder which results more than the actual values. Probably, this might be come from the coefficients which represents of basin characteristics. Snyder method is to make calculations taking into account the geometry of the basin. However, the method is not suitable for smaller basin than 30 km^2.

However, SCS is one of the recently developed methods having simple triangular shape to determine to runoff from rainfall for smaller areas than 30 km^2 in USA. In the test, SCS gave minimum values for same area. Thus, type of land use and curve number must be chosen very carefully.

Rational and Mac Math method are used widely in the country and abroad. While Mac Math gives good results for calculation of channel capacity at all sizes of area but, it does not give good results at hilly and uneven lands. Rational method is more suitable for small areas in cities which is smaller from 25 km^2. The rainfall intensity related to soil permeability and the coefficient of representing the plant cover in the field should be determine carefully in this m

Mockus method gives results closer to actual values according to Snyder Method. Probably, this is because the calculation is made taking into account the slope of the creek and flow depth.

Because Iszkowski ve Lauterburg methods gave disproportionate and different results than the others, the tests should be repeated in any other basins.

Kirpich method has the triangle hydrograph and the formula is simple and convenient for the application. It is preferred where the slope is higher than 10% and the wooded areas are more than 60%.It could be used safely in case of the absence of withdrawal curve is not significant.

Although, Degree-day method is simple and practicable in calculations of discharge from snow, but wind speed, vegetation, rainfall, soil structure are taken into account with this formula.

As a result, most of the empirical and deterministic methods used in flood flow calculation are based on the characteristics of the river basins where they were tested. Therefore, the hydrological, meteorological, topography, plant cover conditions of basin are the most important issues. On the other hand, the assumptions of formulas, characteristics and coefficients are different from each other. As a result, considering restrictive conditions and properties both basin and equations mentioned above, calculations of discharge should be made.

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Driving Shaft Fatigue Life Determination According to Turkish Mission Profiles

Arif Senol Sener*‡

*Department of Mechanical Engineering, Faculty of Architecture and Engineering, Istanbul Gelisim University, Avcılar, Istanbul, Turkey.

(assener@gelisim.edu.tr)

‡ Corresponding Author; Arif Senol Sener, Department of Mechanical Engineering, Faculty of Architecture and Engineering, Istanbul Gelisim University, Avcılar, Istanbul, Turkey. Tel: +90 212 422 7000, Fax: +90 212 422 7401, assener@gelisim.edu.tr

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Abstract- In this study, a questionnaire was used to determine the average customer usage of the light commercial vehicles in Turkey. Approximately on 50 road routes and on rough roads in Turkey, the fatigue characteristics of the road profiles were measured by a many sensors equipped on LCV (Light Commercial vehicle).This article focuses on defining the general load spectrum of Turkey roads belong to the driving shaft. Rain-flow statistical counting method was applied driving shaft's signals in order to make fatigue comparisons meaningfully and other application. Fatigue analysis of the driving shaft according to MP (Turkish mission profiles) were calculated by using FEA (Finite Element Analysis) and verified by the Palmgren-Miner rule.

Keywords: Customer usage driving shaft, finite element analysis, fatigue analysis, Palmgren-Miner Rule.

1. Introduction

Typical automotive design requirement are include the following: high stiffness, good fuel efficiency, smooth ride and handling, occupant comfort, drive characteristics. These requirements must be achieved along with adequate durability and reliability of the vehicle within the warranty timeframe [1]. Durability deals with the material fatigue. This kind of defect can be encountered on old or high millage vehicles**.** The durability of the vehicles depends on three important parameters: design geometry, material properties and loading environment. One of the parameters of loading environment is road roughness. It is well known that under normal conditions, vehicles are exposed to occasional high loads. It is important to have accurate statistical descriptions of these loads which are often caused by road irregularities [2, 3]. Road quality can vary dramatically from country to country. As such automobile manufactures should set quality and durability design constraints in accordance with customer expectations in the target market. To take preventive action on durability defects, which can occur due to weak design and process, manufactures need accelerated fatigue tests and simulations methods. Durability tests are necessary to adapt vehicle performance to customer expectations [4].

Today, automobile manufactures use four durability test methods: fatigue analysis based on Finite Element Analysis (FEA), test rigs, test benches (one particular actuator test), and a accelerated test tracks. The most popular method is used for the determine load spectrum for the whole life of vehicle is customer usage based methods. FEA-based fatigue analysis can be performed in a very short time period and can provide a convenient design solution [5, 6]. To meet these requirements, an important activity in a modern development process is the use of calculation and simulation at an early stage. Computer aided engineering (CAE) is playing an increasingly important role in predicting vehicle characteristics and simultaneously replacing physical test.

In the previous studies about the driving shaft, in 2011, a fuel cell vehicle's driving shaft was investigated by using high performance lightweight materials [7]. In 2006 a fatigue failure of a rear axle shaft of an automobile which has 9 years old was examined in order to understand if the failure was caused by fatigue failure by Asi.O[8]. In 2009 maximum torsion capacity of a hybrid aluminum/composite drive shaft was examined with FEA by S.A.Mutasher [9]. In 2007 fracture and stress analysis of a universal joint and a drive shaft of an automobile power transmission system was done with FEA and by H.Bayrakceken et. al. [10]. In 2008 a failure analyses of elevator of driving shaft was analyzed using FEA and the reason of the fatigue failure was determined by A.Goksenli and I.B.Eryürek [11]. In 2008 fatigue stress fracture of a drive shaft of a caterpillar was searched by FEA and also metallographic examination in

order to determine real cause of the damage by E.Rusunski et al. [12].

One example of a customer usage study; Tractor usage aim on wet and dry ground and also tractor usage for agriculture and non-agriculture and regional usage aim distribution were determined in India from E.T.E.C. (Eicher Tractors Engineering Centre) and A.R.I.A. (The automotive Research Association of India [13].

Another example is a customer usage study performed by FIAT Co. for Brazilian and Italian markets. As it is well know that Brazil and Turkey haven't special proving ground in order to make test on standard fatigue road for the development of the new car models. During the research FIAT Co. compared proving ground profiles effects of Italy and Brazil's public roads including customer usage effects on the vehicles by using frequency based fatigue life [14].

The next example is of a customer usage study was done by FIAT Co. AMOA (automobile mode of operation systems) on Ritmo 60 and Tipo1372 DGT [3, 15].

And one of the other example is of customer usage study was performed by TOFAS A.Ş. for defining Turkish customer vehicle usage profile and fatigue characteristic effect of Turkey's road profiles on a light commercial vehicles[16,17].

Differences of this study;

• Firstly, Turkish customer automobile usage profiles were determined by questionnaire method. Holiday time and the distance lived from the home which is the one of the parameter of the questionnaire has been done by FIAT in 1993[3, 15]. FIAT had accepted the holiday concept as the interval of holiday more than three days and if the distance is far away more than 300 km from the residence area. In our study the holiday concept is restudied and holiday interval was decreased from one week to three days and the holiday distance was accepted 300 km from the residence area were applied on the Turkish customer in 2001 as a questionnaire[16].

• Secondly, on the other studies road roughness fatigue characteristic effects on the vehicle were acquired both from the public roads (city roads, intercity, mountain and highway) and also mixed some special proving ground data. But in this study, the road roughness data were acquired only from public roads and instead of special proving ground effects very heavy village roads including mostly potholes and sharp curves and rocked bad road profiles were added due to the lack of standard proving ground in Turkey.

The road fatigue characteristics were measured totally from one city to another city since to make a comparison on different roads effect. The design of test roads is extremely important for accurately simulating vehicle life. In the following section a methodology for defining test roads for a light commercial vehicle is explained.

2. Methods and Analysis

Durability tests for a vehicle or component must simulate the entire load spectrum (MP: mission profile, Turkish general road characteristics) experienced during normal usage. This means that the load spectrum must cover all anticipated tasks and conditions during the lifetime of the vehicle [18, 19]. The service life of a vehicle component largely depends on the loading conditions during usage [19].

For design and test purposes, it is necessary to define a representative loading spectrum, which should be used for design evaluation as well as for derivation of a load spectrum for durability tests [18,19]. Today there are two methods used to determine customer usage are the questionnaire and black box method.

2.1. Black Box Method

The black box system is based on an electronic "black box" which has the same size as a car radio set and is trouble free for the users which are fitted to a number of cars of preferential users selected by stratification criteria. A lot of data were measured and directly recorded in digital form on static storage [3, 15, 20].

2.2. General Description of a Questionnaire Method

This method implements a large telephone survey designed to acquire information about the distribution of route types (city, extra urban, mountain, highway) the distribution of loads (driver without loads, driver and half load, driver and full load) customer education level, and the purpose of vehicle usage etc.**[**3,19,21]. After acquiring the questionnaire results, a road test simulation is performed to collect data with an equipped vehicle or several equipped vehicles on public roads and special proving ground, during various maneuvers (braking, curving, accelerating), during power generation (engine and transmission components, in various location, on various type of roads (city, intercity, mountainous, rural), and by a test driver or multiple test drivers [3, 19]. Then the collected row data are subjected to data processing like spike, filtering, manipulating etc. Then the signals are divided according to road type and load condition. Data processed road excitation signals are transformed into normalized unit values. Then each road signal is subjected to statistically counting method 3D matrix or 2D range. So it is possible to make comparison of each road signal for each sensor. By multiplying the questionnaire with road type and target km, it is easy to form the target mission profile. The target mission profile (which consists of road excitation signals taking into account 90^{th} percentile distribution of customer automotive usage, load, and the target of MP for the light commercial vehicles is 200 000 km) is obtained for each sensor [16]. The methodology is based on the following principle, if the same inputs are reproduced, then same damage will occur [21].

After forming MP, it is then possible to find mixes of tracks or rig drivers that match to the inputs for accelerated test including track or test rig that are corresponding to the same damage effect of MP. If the same inputs are maintained, matrix calculation of various forms will provide a scheme for assessing the mixture of road excitation signals, and for optimizing the test length or test time.

A [X1] + B[X2] + C[X3] +……..+Z [Xn] = [Y]

Where;

A, B, C ….Z : Multipliers of test data

[X1], [X2]…….. [Xn] : Matrix of test measurements

[Y] : Matrix of customer target measurements.

This can be interpreted quite easily as: A times track X1, followed by times track X2, and so on, so that it gives the same effect as y of the target [21].

3. Application Examples

In this study for road test acquisitions one FIAT Doblo Passenger car LCV was selected and it was designed for transportation of goods and passengers. The algorithm of the study is presented in Fig.1

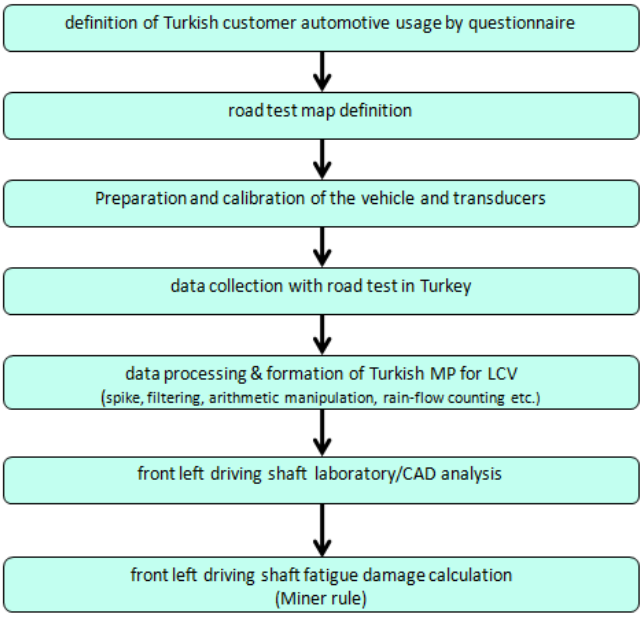

Fig. 1. Algorithm of the study

3.1. Definition of the Turkish Profile –Questionnaire *Application.*

Because the questionnaire method allows a faster data collection, provides flexibility on data elaboration and reduces cost compared to the black box method. As such, it was the method of choice in this study. The Turkish customer usage profile of a LCV that is used for transporting both goods and passengers was developed based on a questionnaire administered to Turkish customer with my support and also with the support of automotive dealers representing the LCV manufacturer.

3.2. Definition of the Turkish Profile-Definition of Road Map

The test road map represents 90 % of customer usage in Turkey. Roads were divided in four groups: city road usage was found to be more common around the Istanbul district; Mountain roads were more common in the Black Sea region. Intercity roads, which include hot climatic and curved road condition, were found around the Mediterranean Sea. Roads in Central Anatolia were characterized by high altitudes, hot temperatures, and long distances between cities. For the highway road characteristics Istanbul-Ankara and Adana – Gaziantep roads were subjected to data acquisitions. Those test roads in the road test map was designed taking reference of the sale percentages of LCVs according to region, customer complaints, previous model experiences, climatic conditions, and geography [16, 17]. The test road map formed taking reference above information for data acquisitions is presented in Fig.2.

Fig. 2. Road test map

3.3. Definition of the Turkish Profile-Data Acquisition to Define the Mission Profile Target

In this study, the measurements were carried out with a vehicle equipped with sensors and driven over customers on chosen roads by an expert test driver and an engineer at full loads. For data acquisition and fatigue simulation, a vehicle was equipped with load transducers, two strain-gauges on the leaf spring, one strain-gauge on driving shaft, and one strain-gauge on the steering wheel rod. The driving shaft torsion torque loads created by maneuvers, breaking and acceleration were measured by strain-gauges on the driving shaft. The mounted strain gauge on the driving shaft in order to measure torsion torque data is demonstrated Fig.3.

Fig. 3. Strain-gauge mounted on driving shaft in laboratory

The strain-gauges calibration on the front left driving shaft is presented In Fig.4 and the other transducers, sensors and strain-gauges were prepared, calibrated and analyzed in the laboratory before being assembled on the car.

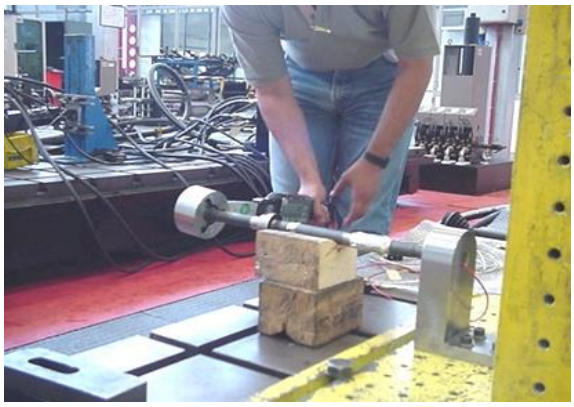

Fig. 4. Strain-gauge mounted on driving shaft in laboratory

3.4. Data Processing

For fatigue data collection at time domain, we could not measure external loads directly. Instead of that we measured their reactions at certain points of vehicle parts [22]. The collected signals were processed by spike analysis, frequency analysis, filtering, arithmetic manipulation and statistical counting operation [23]. The algorithm of the data elaboration process is presented in Fig.5

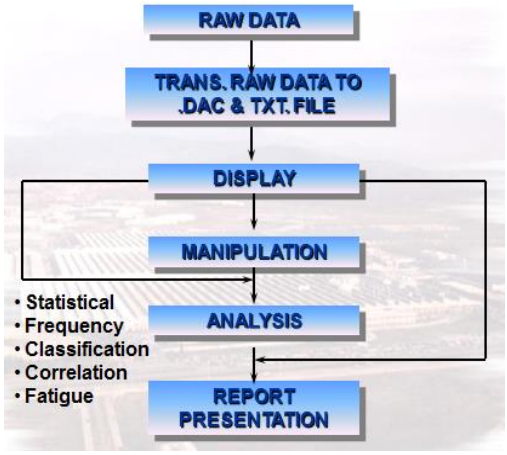

Fig. 5. Algorithm of the data elaboration process

Spike Analysis: During data acquisition some ‘’spikes’’ which were occurred due to environmental and physical factors, were eliminated by visual and statistical methods [23]. A sample spike elaboration analyses of the signal is presented in Fig.6.

Fig. 6. Algorithm of the data elaboration process

Filtering: As it is known that vehicle suspension parts frequency range of interest for fatigue analyses is between 40 Hz and 60 Hz. For road simulation, it is generally accepted that excitation over 100 Hz can be neglected [24].]. Above 100 Hz frequencies in the original data were removed by means of a low-pass filter is presented in Fig.7[16,17,23,24].

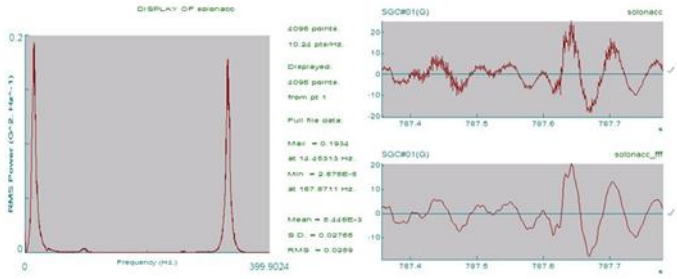

Fig. 7. Low- pass filter application on the driving shaft signals

Arithmetic Manipulations: In this study, acquired each test data which is not useful for fatigue life calculation is extracted before the vehicle movement [23].

Statistical Road Excitation Signal Counting: The road signal is formed by random and stationary signals that are time- varying. Time –varying signals should be converted to an equivalent value independent of time for comparison. The statistical counting method was applied to achieve this conversion [25].The driving shaft strain-gauge data were reduced to foreseen 200.000 km MP values using the rain-flow statistical counting method taking into account mean amplitude of the driving shaft torsion data [25,26].

Forming Mission Profile Target: As the each acquired data had different lengths, the each measured data was normalized to convenient distance in kilometers (i.e., 1 km or 10 km) in order to compare and extrapolate for MP [15, 16, 21]. Each normalized measurement was classified according to road type (city, intercity, mountain, and highway), each road type was averaged within its class. Then each classified measurement was extrapolated to the estimated target km of MP and then multiplied by the percent Turkish customer usage distribution which the given road type based on the questionnaire. The histogram of driving shaft torsion data MP (Turkish customer automobile usage fatigue character-istic of driving shaft for 200.000 km) is showed Fig. 8.

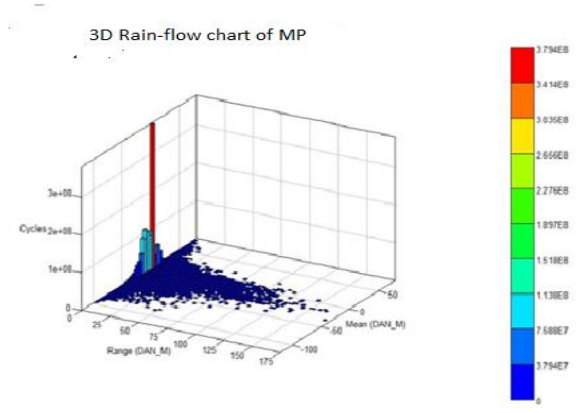

Fig. 8. Driving shaft Mission Profile rain-flow histogram (200.000 km)

4. Simulation of Experimental Data by Finite Element Analysis

4.1. Driving shaft CAD model

The CAD model of the driving shaft was designed in SOLIDWORKS software program is presented in Fig.9 [27].

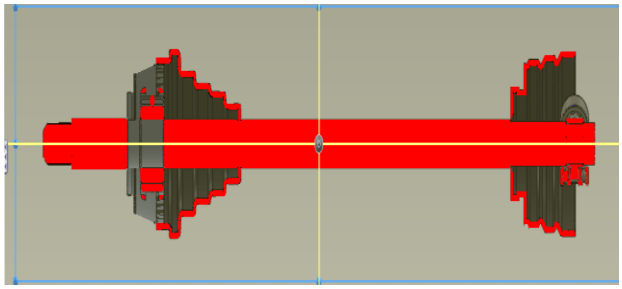

Fig. 9. CAD model of driving shaft

Then 3D CAD model of the driving shaft was exported to ANSYS program to perform FEA analysis. 3D CAD model of driving shaft was formed from 155187 tetra hexagon elements and 253739 nodes is presented in Fig. 10 [28].

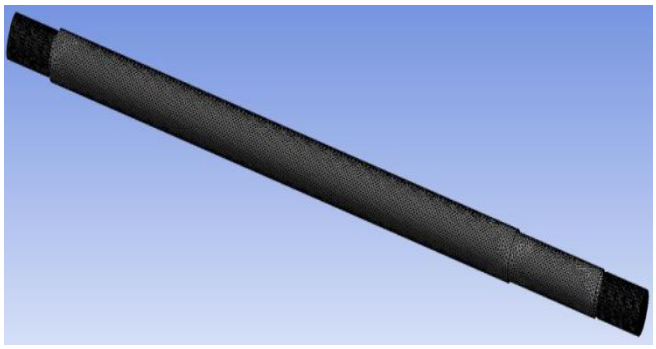

Fig. 10. FE Model of the driving shaft

4.2. Boundary Condition

The boundary condition of driving shaft is presented is presented in Fig.11. As it can be seen from the picture, the red rotating arrow demonstrate the applied torsion torque from the gearbox side which is allowed free only rotation axis while the other wheel side of the driving shaft teeth which is demonstrated with blue arrow is nailed tightly crosshead with bearing inside of spindle which is connected to axon with a bold is demonstrated and the fixed point was not allowed freely both rotation and shift every three axis [28].

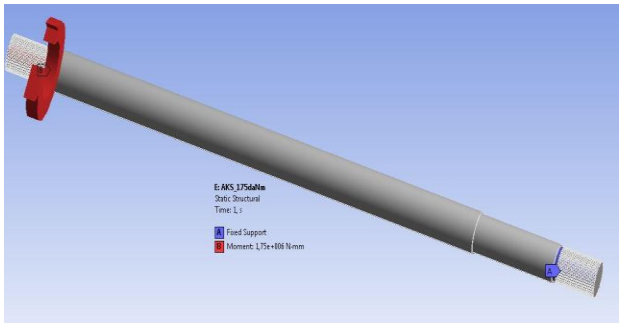

Fig. 11. F. Boundary conditions of the driving shaft

4.3. Static and Fatigue Analysis

The linear static analysis of the driving shaft was executed using the most critical load that was acquired during road tests in Turkey is shown in Fig.12 [16].

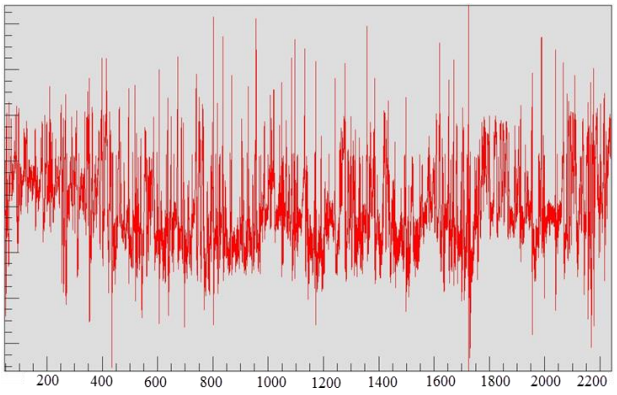

Fig. 12. Critical road data torque -time signal of driving shaft

For the statistical analysis of the driving shaft, the maximum load data, measured during the road test, was applied as torsion at side of the gear box approximately 175 daN.m by using the FE model. After applying 175 daN.m torques in torsion axis 0.0174 $\mu\gamma$ angular strain was derived is presented in Fig.13. At the same time the maximum shear stress was found 1397 Mpa at node 5796 according to the von-Mises method using the most critical load condition in the linear static analysis. [29].

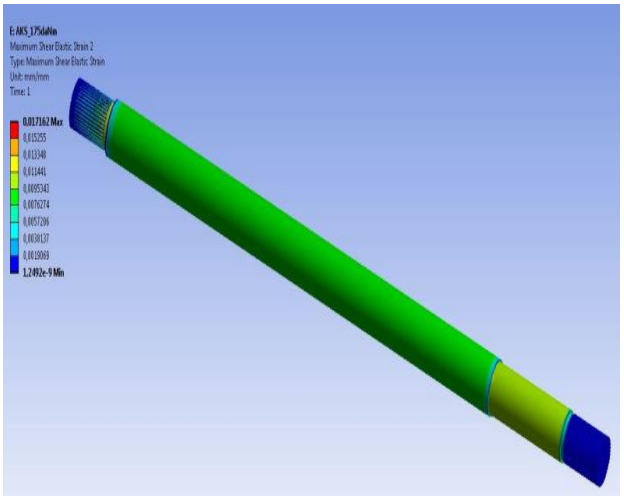

Fig. 13. Static strain analysis of driving shaft according to 175 daN.m torque

The driving shaft real bench test and CAD static analysis strain values comparison is presented in Fig.14. As it can be seen from the graphics that vertical axis demonstrates physically applied torque loads whereas axial axis demonstrates derived angular unit strain on the driving shaft in laboratory and CAD during calibration test. Square symbol demonstrate us physically applied torsion moment on the driving shaft in lab while triangle symbol shows us the CAD static analysis result after applying same loads on the FE model of driving shaft. When 100 daN.m is applied 0.00872 $\mu\gamma$ by the physical test, 0.0098 $\mu\gamma$ by the computer analysis test were measured

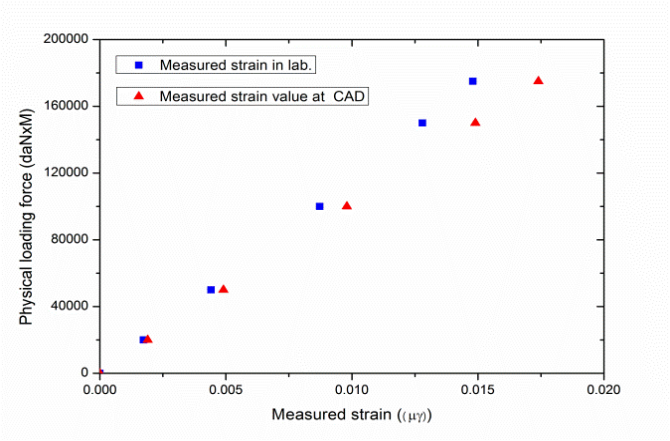

Fig. 14. Driving shaft real bench test and CAD static analysis strain values comparison

The maximum stress is much lower than the actual yield stress of the driving shaft material yield stress. The S-N method was preferred because the values obtained of the data of different kind of the roads in Turkey are much lower than the material yield stress [16, 30]. The Wohler line S (stress) - N (number of cycles) of the material characteristics of the driving shaft is shown in Fig. 15.

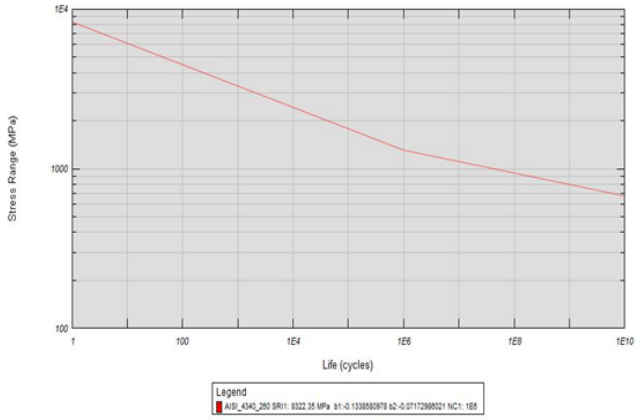

Fig.15. S-N curve of the driving shaft material

4.4. Palmgren-Miner Analysis

Miner's rule is one of the most widely used cumulative damage models for failures caused by fatigue. This linear damage concept in a fatigue setting by considering the situation where a component is subjected to n_1 cycles at alternating stress σ_1, n_2 cycles at stress σ_2, …, n_N cycles at σ_N . From the S-N curve for a material, then it is possible to find the number of cycles to failure, N_1 at σ_1 , N_2 at σ_2 , …, N_N at σ_N.It is reasonable in this case to let the fractional damage at stress level σ_i be simply n_i/N_i ,so that the Palmgren-Miner rule would say that fatigue failure occurs when $\sum_{i=1}^{N} \frac{n_i}{N_i} 1$ [31].

In this study the Palmgren-Miner rule was applied.

5. Results

From the questionnaire Turkish customer automotive usage for LCV is defined. When the derived data are compared to one of the European countries, the major difference is found in the amount of city usage, which is 50 % in Turkey. The primary purpose of aim of usage of LCV in Turkey is for work-work travel. Table 1 shows Turkish customer aim of usage of LCV [16].

Table 1. Turkish customer aim of usage of LCV

Home-work-home	29 %
Work to work	55 %
Shopping and leisure	4.7 %
Weekend	5,4 %
Holiday	5,5 %

The 2D Turkish mission profile for driving shaft data in horizontal axis cycle and in vertical axis torsion torque is presented in Fig.16. From the MP test in Turkey 175 daN.m like the maximum torque load is reached.

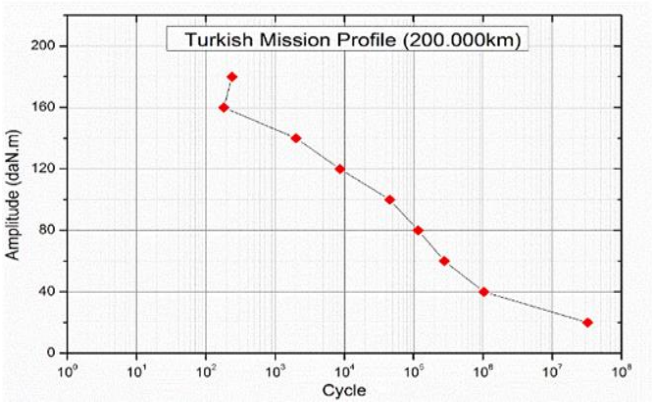

Fig. 16. Turkish mission profile driving shaft data for 200.000 km

Fatigue CAD analysis of driving shaft in terms of fatigue life is shown in Fig.17. Fatigue damage isn't occurred.

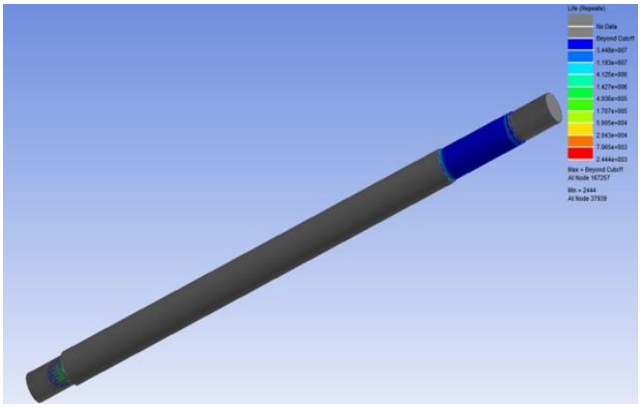

Fig. 17. Fatigue life of driving shaft applied MP data 200.000 km

6. Conclusion

In this study, Turkish customer usage profile was developed based on a questionnaire handed out to Turkish light commercial vehicle users [8]. A comparison of LCV automobile usage between a European country and Turkey was presented. This revealed that the Turkish customers use this type of vehicle for city driving twice as much as typical users in a European country [16].

The primary purpose of light commercial vehicle usage in Turkey is work-work and work-to-home travel. A mission profile of LCV usage specific to Turkish drivers was developed. After processing, classifying and normalizing different signals, a mathematical mission profile (200.000 km for a typical Turkish customer) was calculated. Fatigue road test were performed by applying computer aided fatigue method to data measured by several vehicle mounted sensors [16, 17].

Based on this analysis, critical force and stress ranges have been defined and recorded in a database for future reference during development projects. Tetra and hexa type 3D elements have been used in FEA models. Tetra type elements were found to give more precise results in terms of frequent and geometrical aspect for the teeth of the driving shaft. The linear analysis method that is used in virtual analysis of the structure gave more precise results for this kind of driving shaft.

Due to the fact that the number of cycles was quite low, and it was seen that the S/N fatigue method was more suitable. It has been verified that there was no fatigue damage occurred on the driving shaft after applying the Turkish customer profile.

It has been observed that computer aided analysis can be used as an alternative for laboratory tests because the results that were obtained from both methods were quite similar. Based on these results, using computer aided calculation methodologies it can be seen that it is both cost effective and helpful to develop better and market specific products. The results of this study can also be used for developing new automobile models, before construction of real prototypes and pre-serial production cars..

Acknowledgements

TOFAS A.Ş. is acknowledged for supporting this research.

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Planning and Design Principles of Transmission Line in Water Supply Project

Necati Gulbahar*‡

*Department of Civil Engineering, Faculty of Engineering and Architecture, Istanbul Gelisim University, Istanbul, Turkey.

(ngulbahar@gelisim.edu.tr)

‡ Corresponding Author; Necati Gulbahar, Department of Civil Engineering, Faculty of Engineering and Architecture, Istanbul Gelisim University, Istanbul, Turkey, Tel: +90 212 422 7020, Fax: +90 212 422 7401, ngulbahar@gelisim.edu.tr

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Abstract: Water is an essential substance for human life and living things. It is not substance for the life, but also energy input for agricultural and industrial production. In addition to, it is needed for human daily activities and environment. Water is taken to a place where people need by with transmission lines in water supply project. A transmission line is designed according to requirements, topographic conditions, engineering principles and economic criteria. Transmission lines are large scale projects which planned and projected by public organizations which are DSI, Provincial Bank and Municipalities. Although they are competent and experienced; some problems have been observed in water supply projects such as; lack of future plan, expropriation problem, improper pumping station, incapacity, inefficiency, pollution, poor quality, necessity, inadequate itineraries, too long lines. To avoid these problems, first future development plan for cities should be made and carried out without compromising. Next, the detail study should be carried out for each project from engineering, environmental and economic aspects. In this paper, these issues were examined and discussed to take attention to some important points in planning and designing of transmission line for the application.

Keywords: Transmission, water supply, planning, design.

1. Introduction

Water is the basic material for humans and other living things they need for survival of them. Besides, water is a source of energy that people need, at the same time, it is an essential input for agriculture and industry. Furthermore, water is a determining component of environment. These issues emphasize the importance of water that cannot be discussed. However, the determining factors of policies of societies in history can be listed as water, food and energy.

In the history, the aqueducts instructed by Romans are a transmission line in terms of engineering in Istanbul. Water requirement of Istanbul was supplied from water resources in Belgrade Forest which is 33 km from the city.

Presently, the water requirement of Istanbul is supplied from Melen Dam on the Melen River in Duzce Province with Melen transmission line which is 185km length and with the diameter 2540-3000 mm. The project having four stages and will supply totally 34.2 m^3/s discharge until the year 2040. (Fig. 1)

Similarly, the water requirement of Ankara is supplied with a transmission line from Kesikkopru Dam which is 128 km length with the diameter1400-1600mm Steel CTP pipe.

Another transmission line, water conveyed Alakopru Dam in Anamur from Turkey to the Gecitkoy Dam in Turkish Republic of Northern Cyprus (TRNC). The transmission line which is the first in the world covers four stages which are Turkey coast, sea crossing, TRNC coast and country network. It is totaly106 km length with the diameter of 1600mm high density polyethylene pipe with the discharge 2.38 m^3/s. (Fig. 2-Fig. 3).

The need of society is increasing day by day due to population growth and technological advances as a result of these natural resources are rapidly consumed. Worse, resources have been polluted which contributes to the amount of reduction. Actually, water resources are a concrete sample for this situation.

A transmission line is a line which is transmitting to take water from a source where needed in any water supply projects. There is no water distribution from this line. İf this line fails for any reason, the area will not be supplied. Therefore, the double or triple line should be constructed according to needs. İn order to transport water from long distances safely, transmission lines should be constructed in accordance with engineering, environmental and economic criteria. Transmission line is not only used water, but also oil

and gas. As compared with other forms of transport, transmission line is much safer and cheaper than all of types transport.

Transmission lines are mainly constructed in two ways which are free surface and pressure systems due to topographical, engineering and economic reasons. İf resource is higher than the reservoir, transmission is designed under gravity. Otherwise, pumping is needed. There are several types of free surface transmission systems. İt is preferred the optimum type according to topographic and economic conditions. The transmission line can be classified as follows;

a. Free surface systems
- Open channel
- Aqueduct
- Tunnel
- Galleries

b. Pressurized systems
- Gravity
- Pumping
- Gravity- pumping

In this paper, a transmission line as a part of water supply project will be discussed and some important points will be emphasized for the purpose of better design in the application.

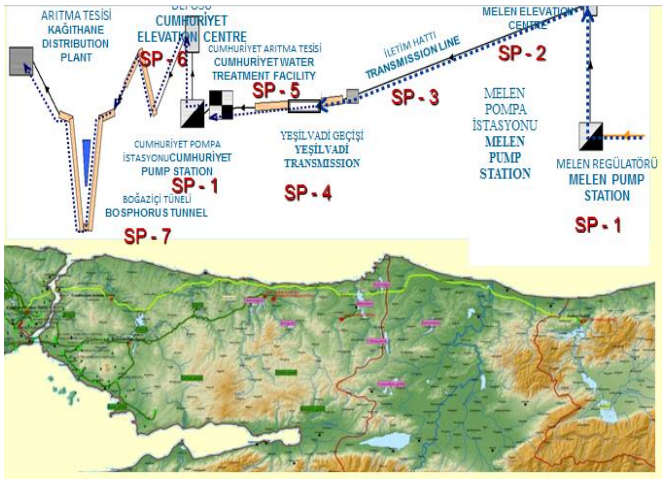

Fig. 1. Melen project plan and transmission line [2]

Fig. 2. Plan of transmission line between Turkey and TRNC [6]

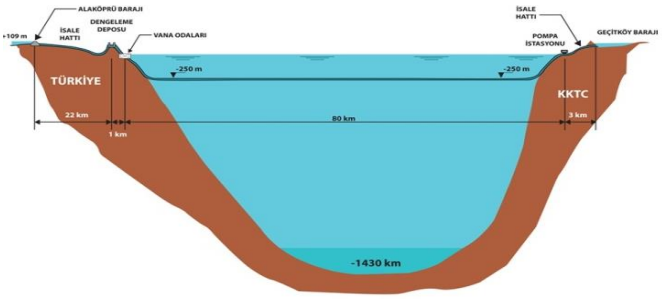

Fig. 3. Profile of the transmission line between Turkey and TRNC [6]

2. Design principle of transmission line

Mainly, transmission lines have been designed in two ways which are gravity and pumping systems. Gravity Systems, The most important point in this method is to determine piezometric line carefully. The piezometric line is indicated as $\mathbf{P}/\gamma$ **+z** which are pressure head and geometric elevation that is provided with the difference between the static line and the pipe. In case of water resource is at the higher elevation than the storage reservoir in the city, the water can convey by the gravity. First an itinerary is determined next ground and pipe profile is designed. Then pipe diameter is determined based on piezometric line and discharge. Head loss should not be bigger than piezometric head which is the difference between piezometric line and pipe level.

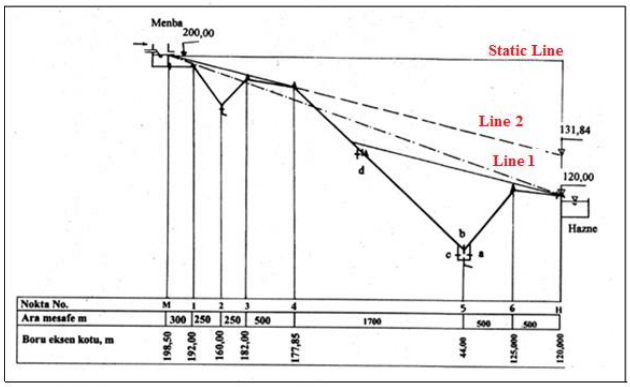

Fig. 4. Gravity transmission line designed by classical method [10]

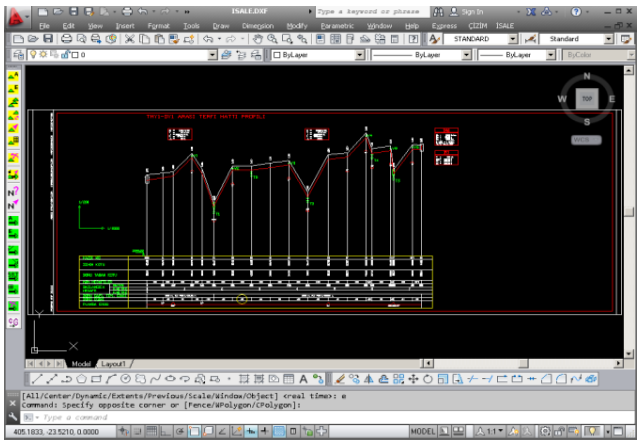

Fig 5. Transmission line designed by computer [4]

From the Figure 4, Line 1 is not acceptable due to pressure decrease or free water surface occurs, but Line 2 is acceptable because operating pressure is at designed level, which can be easily adjusted by valve.

In a pumping System, determining of the manometric head is the most important part that the pump gives energy to water by converting mechanical energy to hydraulic energy. Manometric height must cover all of head losses and difference in geometric elevation between resource and reservoir including efficiency of pump and motor.

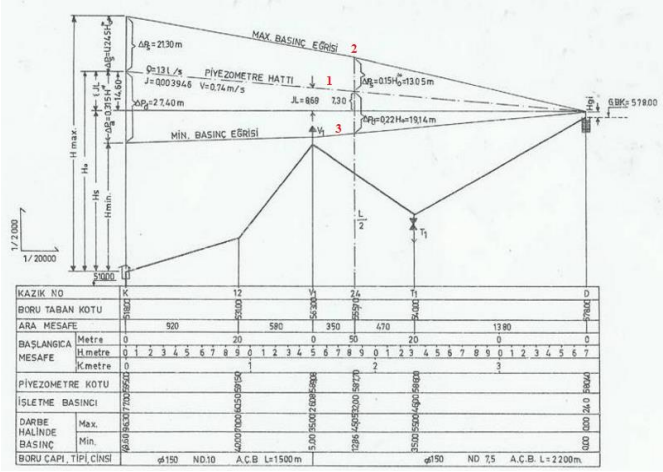

Fig. 6. Transmission line by pumping with classical method [12]

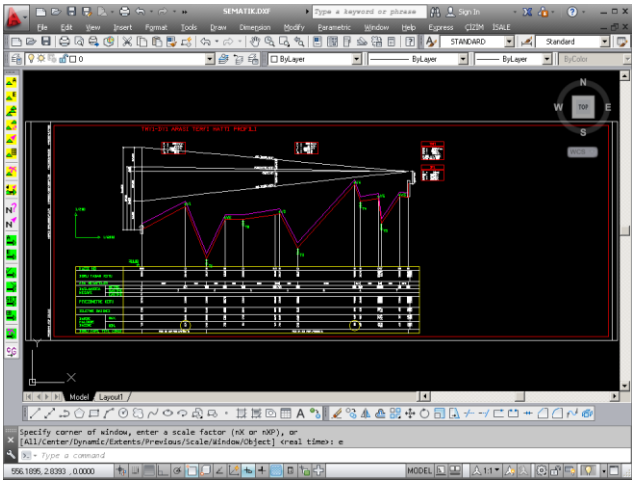

Fig. 7. Suppression and depression calculated by computer [4]

Suppression and depression pressure occur which damage to pipe system in a pumping and it must be calculated. In case of energy cut off, water mass in the pipe first stops, then flows with the high velocity to the pump. This is called as water hammer. At the same time, behind the water mass in the pipe creates a suction which is called depression. This event may also occur more slightly when valve is suddenly closed According to physical conditions, air tank capacity should be calculated and put in the system for reducing the over pressure. Pumps are connected to each other parallel and series with reference to the requirements and conditions. Generally, besides operating pumps, one of them is kept as a spare or stand-by. (Fig. 8).

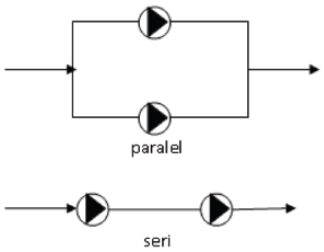

Fig 8. Series and parallel connections [7]

Transmission lines may have curve in some parts of lines. This is applicable with flexible material easily. However some formulas may be used for calculation of minimum radius of curve. Although, 1m depth soil may be eliminated harmful effect of external forces, this can be identified by various formulas.

3. The elements of a sustainable water supply and sewage systems

The basic requirement of sustainable water resource management is that water is taken from nature and given back to nature at least with the same quality with reference to Bruntland report. Therefore, it should be considered as a whole to water supply and sewage system design in any project. Such a system is given in the following schematic layout. (Fig. 9).

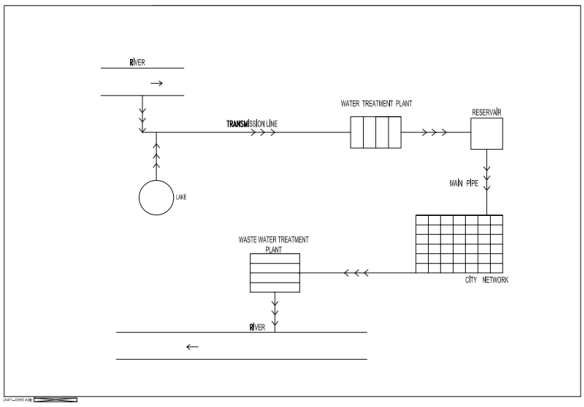

Fig. 9. A sustainable water supply system

From the Figure 9, first surface and underground water resources are collected and transmitted to water treatment plant with the transmission line by means of pumping. After the treatment, it is conveyed to reservoir with transmission line. Next, water is taken from reservoir to the city network with the main pipe. Finally, the outflow water from the network is defined as waste water which should be conducted to the river after treatment process.

4. Points to be considered for planning transmission line

In Turkey legally, authorized government agencies regarding water supply and sewage system are DSI, Iller Bank and municipalities. These institutions carry out planning and designing works of infrastructures in cities and rural areas according to the technical regulations which have developed by their institution. The technical regulations of

DSI will be based on here. Some important items for necessary in designing of transmission line according to the Technical Regulations of Drinkable Water of DSI are summarized as follows;

- Transmission lines should be the shortest line having the highest elevation as possible
- Transportation should be easy and necessary structures must be less
- Flood and landslide risk should be less and far from the river bed
- Pipe diameter selection will be done by 35 years of economic analysis and discharge at that time
- Plans will be the 1/1000 and 1/2000 and the profiles 1/200 and 1/100
- Polygon points, some points and angles will be shown.
- The distance and intermediate distances will be displayed in plan and profile
- The calculation of control and measuring structures will be made separately
- Pressure will be broken with structures if hydraulically is possible
- Air accumulated at peak point in the line will be evacuated with chimney if possible
- Water discharging valve will be put at the lowest point in the line
- Trench depth will be 1m up to 2000 mm and over 2000 it is 1.25m
- The anchoring block will be constructed for stability at sloping areas
- Preventive measures will be taken at the landslide areas
- The pipe will be run under the pressure given by the factory for safety
- Calculations will be made based on static pressure for systems operating with gravity

Except mentioned above, some additional points given at the following that is thought to be useful

- Velocity of water should be V_{min} =0.5 m/s and V_{Max}= 3m/s for pipes and V_{min}= 0.5 m/s and V_{Max} = 2m/s for open channel.
- Cost of drinkable water and waste water treatment systems should be included to the total costs
- Calculations of water needs should be made according to the Provinces Bank method
- Gravity system should be preferred even though expensive by 25%
- Operating Pressure must be p_{min}.= 30 m and P_{max}.=80 m
- At sloping land for uphill elevation will be 0.002 and down-hill elevation will be 0.005
- The cost of 1 m^3 of water should be determined at the end of this calculation

5. Works for transmission line projects

In a water supply project, besides hydrologic and hydraulic study, some certain studies related to construction such as excavation, filling, formwork, concrete, all kinds of work, are available. These are gradual work that each stage is a continuation of the previous stage. Works are known at schedule when and how to do is going to be done. However, the only transmission line works were examined in this paper.

According to technical regulations of the drinking water of DSI, the following works related to the transmission line should be carried out and be prepared in a computer;

- General layout
- Transmission line plan
- Transmission line profile
- Schematic profile of transmission line
- Catchment project (Plan, Profile, Formwork Plan)
- Preservation area project
- River gateway, anchoring block, preservative wall
- Energy transmission line project

According to the above mentioned Regulation of DSI, depending on the gravity or pumping transmission, the following calculations must be done;

- Hydrologic calculations
- Hydraulic calculations
- Moto-pump calculations
- Anchoring block calculations
- Static and reinforced concrete calculations
- Suppression, depression, air boiler calculations
- Bill of Quantities for only engineering structures
- Structures of measuring and control
- Bill of Quantities (BOQ)
- Calculations for other works

Additionally, it is suitable to add to the calculation the following items;

- Excavation-Filling
- Traffic load

6. Equations used for hydraulic calculation

Mainly, continuous head loss and local loss calculation should be made in transmission line. Calculation for the engineering structures should be considered as the local loss and added to it.

For the gravity pipelines, Continuity, William-Hazen, Darcy-Weisbach equations or Moody diagram can be used. In pumped line, pump power, suppression, depression and air boiler capacity must be calculated separately. For open channel, Manning and Darcy-Weisbach equations can be used. Important formulas for hydraulic calculations are given at the following;

William-Hazen : $V = 0.85 . C . R^{2.63} . J^{0.54}$

Continuity : $Q = A.V$

Local loss : $h_{ky} = k. \frac{v^2}{2g}$

Power of the pump : $N_p = \frac{\gamma . Q . H_m}{75 . \eta}$

Manning : $V = \frac{1}{n} R^{2/3} S^{1/2}$

Darcy-Weisbach : $h_k = f * \frac{l}{d} * \frac{v^2}{2g}$

Pressure wave speed : $a = \frac{9900}{\sqrt{48 + k * \frac{D}{e}}}$

Süpression – Depression : $\Delta H = \pm \frac{a * V}{g}$

Curve radius : $R = \frac{L/2}{sin\frac{\alpha}{2}}$

External force acting pipe : $W = \gamma_t . H$

Bresse : $D_e = 1.5\sqrt{Q}$

Where;

N_p : power

γ : Specific wight of water

Q: Discharge

C: coefficent

H_m: Manometric height

η_p ; pump efficiency

η_m ; motor efficiency

v: velocity

f: coefficient friction

l: lenght

d ,D: diameter

n: ruffness coefficient

R; hydraulic radius

S,J: land slope

hk: frictional loss

a: velocity of pressure wave

ΔH: head loss

A; cros sectional area

k : coefficient

k_m =coefficent of material

g= gravitational acceleration

e= material thickness

R: Minimum radius of curve

α = central angle of curve

L= length on the curve between two points

W= soil pressure

γ_t = specific weight of soil

D_e= economic diameter

H= excavation depth

7. Engineering structures in transmission line

Various structures have been used in transmission lines with reference to necessity which are trough, air valve, drain valve, surge tank, air boiler, anchored block, pumping station and special constructions that are briefly summarized below;

- Trough: It is made to reduce the pressure. Water inflows to it, and outflows under the gravity force.
- Air valve: It is used at the top points of the line for evacuation air when the pressure in the pipe decreases.
- Drain valve: It is placed at lowest points of the line and used to drain the water when needed
- Surge tank: It is used for preventing pumping pressure fluctuations occurring in the pipe line.
- Anchored block: It is placed when pipeline passes through on slope areas or dynamic forces in the elbow of pipe to prevent separation from the ground.
- Pumping stations: It provides energy to water. It is needed when the pipe lines which is not run under the gravity.

- Water treatment plant; It is needed to improve water quality with reference to drinkable water standards.
- Special construction: It is needed when the pipe pass through such as; swamp, lake, river and sea.

6. Pipe material

In order to select pipe material, various factors have been considered such as; chemical properties of water, properties of the alignment, strength, lifetime and economic criteria are considered**.** Determining pipe material thickness, the operating pressure, external pressure, and water impacts should be taken into account. Pipes have been made from different materials such as; steel, cast ıron, ductile, poly ethylene (PE), poly vinyl chloride (PVC), glass fiber reinforced pipe (CTP) and concrete. Specifications of these materials are briefly given as follows (Karadogan, 2010):

Steel: High strength, fracture-proof, lightweight and economic but it needs a protective coating.

Cast Iron: Corrosion-resistant, medium strength, durable, more thickness, heavy, fragile against impact

Ductile: High strength, less fragile but imported material

PVC and PE: Strength good, not economic in large-scale, PE flexible but PVC non-flexible.

CTP: Composites pipes that are made using non-metallic chemical substance. Good strength, corrosion resistance but not economical

Concrete: less strength, fragile for impact and heavy

8. Economy of transmission line

Identifying of the optimum diameter in a transmission line is very important. If it is taken the great diameter, the cost of the line increases in that case head losses is reduced. If small diameter is selected, the cost of the line decreases, but this time head losses increases that increases energy cost of the motor and pump power. This situation is shown at the following schematic graph in Fig. 10. From the figure, the number 1 shows annual expenses, the 2 is related to construction cost, the 3 shows the total cost. The optimum point is at D_e. However, at the planning stage Bresse formula can be also used for the estimation of economical diameter.

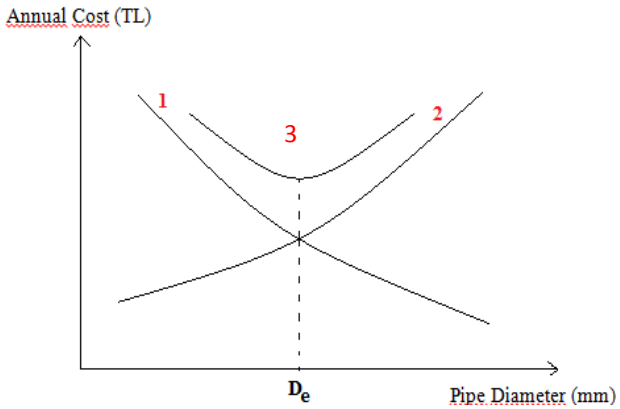

Fig. 10. Economic diameter of pipe [11]

7. Conclusion

As explained above; the most important part of a water supply projects is transmission line. A transmission line may be pipe line or open channel which conveys water to treatment plant. Usually, for drinkable water transmission has been designed due to pollutions and evaporation loss problems. Generally, although gravity system is preferred the topographical conditions are not adequate to convey the water by gravity. Therefore, pumps must be used for energy provide. Another important point, a number of distribution storage reservoirs must be designed to meet hourly variation demand of water depending pressure conditions. Because of the failure of the transmission line for any reason, the line which feeds the area will not have water. It means an interval of social life. Therefore, the place where the line passed through the topography and soil conditions of land should be well studied and itinerary well determined. Likewise, calculations of pipe diameter to meet future requirements are also important. Transmission lines should be as short as possible, which requires less structure and should go up and down with the suitable slope. If possible, it should not be passed through river beds, the marshland and lake. However, if transition is necessary for passing through like these places, then specific projects must be prepared as required. Transmission lines in terms of security must be planned as a double line. From the sustainable view point, the line should not damage to environment and ecological balance should not be disturbed especially during construction and operation period. Finally, the line should be acceptable from economic view point.

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$$C = a + b \qquad (1)$$

Section titles should be written in bold style while sub section titles are italic.

3. Figures and Tables

3.1. Figure Properties

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Figure 1. Engineering technologies.

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