COMPUTATION OF CERTAIN SELECTED DEGREE - BASED TOPOLOGICAL INDICES OF N-DIMENSIONAL OXIDE NETWORK

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ABSTRACT

A topological index is a numeric quantity related to the chemical composition claiming to correlate the chemical structure with different chemical properties. Topological indices serve to predict the physicochemical properties of chemical substances. Among different topological indices, degree-based topological indices would help investigate the anti-inflammatory activities of certain chemical networks. For a molecular graph, G = (V ,E), a general form of vertex-degree-based topological indices is defined as T I(G) = $\sum_{u,v\in E(G)} f(d(u), d(v))$, where f is non-negative real two variable function and d(u) denotes the degree of the vertex. In this paper, we calculated the Harmonic index, Augmented Zagreb index, Geometric-Arithmetic index, Radic connectivity index and Zagreb index of the Oxide network.

Keywords: *Chemical graph theory, Topological indices, Oxide networks.*

INTRODUCTION:

Chemical graph theory has become very beneficial because of its application in mathematical chemistry. In theoretical chemistry, molecular structure descriptors (also called topological indices) are used for modelling physio-chemical, pharmacological, toxicological, biological and other properties of chemical compounds. `According to the IUPAC definition, a topological index is a numerical value associated with the chemical constitution for correlation of chemical structure with various physical properties, chemical reactivity or biological activity. There are numerous molecular-graph-based descriptors. One of the most investigated categories of topological indices used in mathematical chemistry is called degree-based topological indices, which are defined in terms of the degree of the vertices of a graph.

To use a mild expression, today we have far too many such descriptors, and there seems to lack of a firm criterion to stop or slow down their proliferation.

Let G be a molecular graph. Two vertices of G, connected by an edge, are said to be adjacent. The number of vertices of G, adjacent to given vertex v, is the degree of this vertex and will be denoted by dv(G) or, if understanding is not possible, simply by d(v).

For a molecular graph, G = (V,E), a general form of vertex-degree-based topological indices defined as TI(G) = $\sum_{uv\in E(G)} f\big(d(u), d(v)\big)$ where f is non-negative real two variable function and d(u) denotes the degree of the vertex.

SOME DEGREE-BASED TOPOLOGICAL INDICES

Randic or Connectivity index

Historically, the first vertex-degree-based structure descriptors were the graph invariants that nowadays are called Zagreb indices [1-2], However, these were intended to be used for a completely different purpose and these were included among topological indices much later. The first genuine degree-based topological index was put forward in 1975 by Milan Randic in his seminar paper [3].

His index was defined as

$$R = R(G) = \sum_{(u,v)\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$

Randic himself named it branching index, but soon it was re-named to connectivity index. Nowadays, most authors refer to it as the Randic index.

Zagreb indices

Analyzing the structure-dependency of total π-electron energy[4] an appropriate formula was obtained in which items of the form

$$M_1(G) = \sum_{(u,v)\in E(G)} d(v)^2$$

$$M_2(G) = \sum_{(u,v)\in E(G)} (d(u).\, d(v)$$

occurred. It was immediately recognized that these terms increase with the increasing extent of branching of the carbon-atom skeleton. In spite of the lack of practical chemical applicability, scores of papers appeared in the mathematic-chemical literature, in which a variety of mathematical properties of M_1 and M_2 are established. Of these, the remarkable identity

$$M_1(G) = \sum_{(u,v)\in E(G)} (d(u) + d(v))$$

which compared with M_1(G) = hints towards a deeper lying relation between the two Zagreb indices.

Harmonic index

In the 1980s, Siemion Fajtlowicz created a computer program for the automatic generation of conjectures in graph theory. Then he examined the possible relations between countless graph invariants, among which there was a vertex-degree-based quantity.

$$H(G) = \sum_{\{u,v\}\in E(G)} \frac{2}{d(u)+d(v)}$$

With a single exception H(G) did not attract anybody's attention, especially not chemists. Only in 2012, Zang re-introduced this quantity and called it the Harmonic index. His works were followed by a recent paper. No applications of the Harmonic index were reported so far, but, knowing the present situation in mathematical chemistry, such researches are very much to be expected.

Sum – Connectivity index

The Sum – connectivity index was introduced by Bo Zhou and Nenad Trinajstic and it is defined as

$$\mathrm{SCI(G)} = \sum_{\{U,V\}\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$$

A number of properties of the sum – connectivity index has been determined which again are bounds and characterization of graphs of various types, external with respect to SCI details are found in the review.

Atom- Bond Connectivity index

Atom- Bond connectivity (ABC) index was introduced by Ernesto Estrada and it is defined as

$$\mathrm{ABC(G)} = \sum_{\{u,v\}\in E(G)} \sqrt{\frac{(d(u)+d(v)-2)}{d(u)d(v)}}$$

It was shown that the ABC index is excellently correlated with the thermodynamic properties of alkanes [4], especially with their heat of formation. A theoretical explanation for this fortunate property of the atom-bond connectivity index was offered.

Augmented Zagreb Index

Motivated by the success of the ABC index, Furtula etc all put forward its modified version, which they somewhat inadequately named the augmented Zagreb index. It is defined as

$$\mathrm{AZI(G)} = \sum_{\{u,v\}\in E(G)} \left(\frac{d(u).d(v)}{d(u)+d(v)-2}\right)^3$$

Geometric-Arithmetic index

The geometric and arithmetic means, and is defined as

$$\mathrm{GA(G)} = \sum_{\{u,v\}\in E(G)} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

This index was invented by Vukicevc and Furtula and was named the Geometric- arithmetic index. In addition to some mathematical studies of the GA index worth of chemist's interest are its applications to acyclic, unicyclic and bicyclic molecular graphs as well as benzenoid hydrocarbons and phenylenes [5-6].

In this paper, we calculated the Randic index, Zagreb indices, Harmonic index and Sum-connectivity index of the Oxide network.

SILICON OXIDES:

Oxide networks are important in investigating silicate networks. Oxide networks are obtained by the deletion of the silicon nodes from a silicate network. The n-dimensional oxide network is denoted by OX_n and is obtained from the n-dimensional silicate network which is in turn a (silicate) sheet of tetrahedrons. The corner vertices of a tetrahedron are oxygen nodes and the centre vertices are silicon nodes. When all the silicon vertices are deleted from a silicate network, an oxide is constructed. The structure of OX_n should be understood from Fig. 1, where the oxide network OX_2 is shown. The number of vertices in OX_n is $9n^2 + 3n$ and the number of edges is $18n^2$[7-8]. Fig.1 and Fig.2 represent OX_2 and OX_3 respectively. In this section, we calculated the Randic index, Zagreb indices, Harmonic index and Sum- connectivity index of oxide networks.

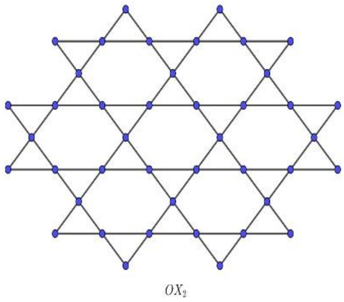

Fig.1

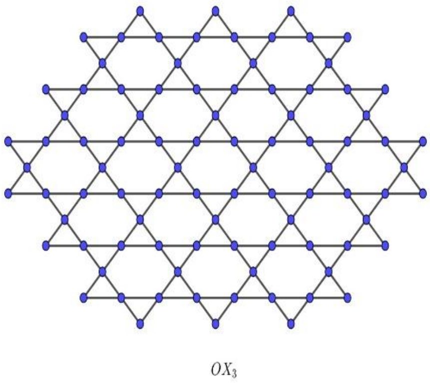

Fig. 2

The total number of vertices of OX_n is $9n^2 + 3n$, and the total number of edges are $18n^2$. The edge set can be partitioned into two disjoint sets as given below.

E_1={e = u~v /d(u)=2 and d(v)=4}

E_2={e = u~v /d(u)=4 and d(v)=4}.

Also $|E_1|=12n$ and $|E_2| = 18n^2-12n$.

MAIN RESULT:

For oxide network (OX_n), we have

a. Randic or Connectivity index $R(G) = \frac{12n}{\sqrt{8}} + \frac{18n^2 - 12n}{4}$

b. Zagreb indices: $M_1(G) = 144n^2 - 24n$

$M_2(G) = 96n + 288n^2 - 142n$

c. Harmonic index $H(G) = 4n + (18n^2 - 12n)\left(\frac{1}{4}\right)$

d. Sum-Connectivity index $SCI(G) = 12n.\frac{1}{\sqrt{6}} + (18n^2 - 12n).\frac{1}{\sqrt{8}}$

e. Atom-bond-connectivity $ABC(G) = 12n.\sqrt{\frac{1}{2}} + (18n^2 - 12n).\sqrt{\frac{3}{8}}$

f. Augmented Zagreb index $AZI(G) = 96n + (18n^2 - 12n).\left(\frac{512}{27}\right)$

g. Geometric-arithmetic index $GA(G) = 12n.\frac{2\sqrt{2}}{3} + (18n^2 - 12n)$

Proof:

Randic or Connectivity index:

$$R = R(G) = \sum_{(u,v)\in E(G)} \frac{1}{\sqrt{d(u)d(v)}}$$

$$= \sum_{(u,v)\in E_1} \frac{1}{\sqrt{d(u)d(v)}} + \sum_{(u,v)\in E_2} \frac{1}{\sqrt{d(u)d(v)}}$$

$$= \frac{|E1|}{\sqrt{8}} + \frac{|E2|}{\sqrt{16}}$$

$$= \frac{12n}{\sqrt{8}} + \frac{18n^2 - 12n}{4}$$

Zagreb indices:

$$M_1(G) = \sum_{(u,v)\in E(G)} (d(u) + d(v))$$

$$= \sum_{(u,v)\in E_1} (d(u) + d(v)) + \sum_{(u,v)\in E_2} (d(u) + d(v))$$

$$= |E1|.6 + |E2|.\ 8$$

$$= 12n.6 + (18n^2 - 12n).\ 8$$

$$= 72n + 144n^2 - 96n$$

$$= 144n^2 - 24n$$

$$M_2(G) = \sum_{(u,v)\in E(G)} (d(u).d(v))$$

$$= \sum_{(u,v)\in E_1} (d(u).d(v)) + \sum_{(u,v)\in E_2} (d(u).d(v))$$

$$= |E1|.\ 8 + |E2|.16$$

$$= 12n.8 + (18n^2 - 12n)\ 16$$

$$= 96n + 288n^2 - 142n$$

$$= 288n^2 - 96n$$

Harmonic index

$H(G) = \sum_{\{u,v\}\in E(G)} \frac{2}{d(u)+d(v)}$

$= \sum_{\{u,v\}\in E_1} \frac{2}{d(u)+d(v)} + \sum_{\{u,v\}\in E_2} \frac{2}{d(u)+d(v)}$

$= |E1| \left(\frac{2}{6} \right) + |E2| \left(\frac{2}{8} \right)$

$= 12n\left(\frac{2}{6} \right) + (18n^2 - 12n) \left(\frac{2}{8} \right)$

$= 4n + (18n^2 - 12n) \left(\frac{1}{4} \right)$

Sum-connectivity index:

$SCI(G) = \sum_{\{u,v\}\in E(G)} \frac{1}{\sqrt{d(u)+d(v)}}$

$= \sum_{\{u,v\}\in E_1} \frac{1}{\sqrt{d(u)+d(v)}} + \sum_{\{u,v\}\in E_2} \frac{1}{\sqrt{d(u)+d(v)}}$

$= |E1|.\frac{1}{\sqrt{6}} + |E2|.\frac{1}{\sqrt{8}}$

$= 12n.\ \frac{1}{\sqrt{6}} + (18n^2 - 12n).\ \frac{1}{\sqrt{8}}$

Atom-bond connectivity index:

$ABC(G) = \sum_{\{u,v\}\in E(G)} \sqrt{\frac{(d(u)+d(v)-2)}{d(u)d(v)}}$

$= \sum_{\{u,v\}\in E_1} \sqrt{\frac{(d(u)+d(v)-2)}{d(u)d(v)}} + \sum_{\{u,v\}\in E_2} \sqrt{\frac{(d(u)+d(v)-2)}{d(u)d(v)}}$

$= |E1|.\sqrt{\frac{4}{8}} + |E2|.\ \sqrt{\frac{6}{16}}$

$= 12n.\ \sqrt{\frac{1}{2}} + (18n^2 - 12n).\ \sqrt{\frac{3}{8}}$

Augmented Zagreb Index:

$AZI(G) = \sum_{\{u,v\}\in E(G)} \left(\frac{d(u).d(v)}{d(u)+d(v)-2}\right)^3$

$= \sum_{\{u,v\}\in E_1} \left(\frac{d(u).d(v)}{d(u)+d(v)-2}\right)^3 + \sum_{\{u,v\}\in E_2} \left(\frac{d(u).d(v)}{d(u)+d(v)-2}\right)^3$

$= |E1|\left(\frac{8}{4}\right)^3 + |E2| \left(\frac{16}{6}\right)^3$

$= 12n.8 + (18n^2 - 12n).\ \left(\frac{512}{27}\right)$

$= 96n + (18n^2 - 12n).\ \left(\frac{512}{27}\right)$

Geometric-Arithmetic index:

$$GA(G) = \sum_{\{u,v\}\in E(G)} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= \sum_{\{u,v\}\in E_1} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))} + \sum_{\{u,v\}\in E_2} \frac{2\sqrt{d(u)d(v)}}{(d(u)+d(v))}$$

$$= |E1|.\frac{2\sqrt{8}}{6} + |E2|.\frac{2\sqrt{16}}{8}$$

$$= 12n.\frac{2\sqrt{2}}{3} + (18n^2 - 12n)$$

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DETERMINATION OF PHYSICO-CHEMICAL CHARACTERISTICS OF ORGANIC LIQUID USING REDLICH-KISTER COEFFICIENTS

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ABSTRACT
The algebraic representation of thermodynamic properties and the classification of solutions are given by Redlich-Kister polynomial equation. This equation can be used to fit activities in two component mixtures over the entire concentration range and to calculate the activities of both components. In the present study, organic liquid with CCl_4 is taken for study. Various parameters for the binary liquid at different temperatures as 308 K, 313 K, 318 K, 323 K and 328 K have been estimated. From these data, excess molar volume, deviation in viscosity, velocity and various excess parameters like adiabatic compressibility, free length, etc are calculated. The values are fitted to a Redlich-Kister polynomial equation $Y^E = x_1 x_2 \sum_{i=0}^{n} A_i (x_2 - x_1)^i$ and the binary coefficients and standard deviations are estimated. From the R-K coefficients, the physico-chemical characteristics of the samples are analyzed and discussed in terms of molecular interactions.
Keywords: Adiabatic compressibility, excess molar volume, free length, Redlich-Kister polynomial.

INTRODUCTION
The chemical and physical of binary and ternary mixtures are important for understanding their thermodynamic behavior. One of the most important considerations is that these properties may provide information about molecular interactions [1-4]. The study of structural packing, the study of shape and the study of size is generally affected by the molecular interactions. Speed of sound studies and related thermo acoustical excess parameters in liquids and liquid mixture are useful in explaining molecular activities with their typical behavior [5]. The Redlich-Kister coefficients generally for the study of interactions among the molecules of liquid specie. The algebraic representation of thermodynamic properties and the classification of solutions are given by Redlich-Kister polynomial equation. This equation can be used to fit activities in two component mixtures over the entire concentration range and to calculate the activities of both components [6].

In the present study an attempt has been made to compute the excess molecular interaction parameters of binary liquid mixtures of propane-1-ol and CCl_4 at different temperatures 308 to 318K in steps of 5K. The experimental density, viscosity and ultrasonic velocity values are taken from the literature [7]. From the literature data, excess molar volume, deviation in viscosity, velocity and various excess parameters like adiabatic compressibility, free length, etc. are calculated. The values are fitted to a Redlich-Kister polynomial equation and the binary coefficients and standard deviations are estimated. From the R-K coefficients, the physico-chemical characteristics of the samples are analyzed and discussed in terms of molecular interactions.

MATERIALS AND METHODS
The chemicals used in this experiment are of analytical grade and used without any purification. The liquid mixtures were prepared by mixing the calculated value of molar concentration in an air tight glass bottles to minimize the evaporation and contamination of the solvent. Speed of the ultrasonic waves in liquid samples has been measured using an Ultrasonic Interferometer (2MHz – Mittal make). The temperature of the liquids in the measuring chamber is stabilized by a water circulation thermostat which maintains the temperature with the minimum accuracy of ±0.2C. The density is measured using a 5 ml specific gravity bottle with experimental liquid immersed in a temperature-controlled water bath. The

viscosity of the liquid samples is measured using an Ostwald's Viscometer which was reported in literature [7].

Redlich-Kister Polynomial

The algebraic representation of Thermodynamic Properties and the classification of solutions are given by this polynomial equation [8-10]. This equation can be used to fit activities in two component mixtures over the entire concentration range, and to calculate the activities (molecular level) of both components.

This method furnishes an immediate distinction between various types of solutions. The excess molar volumes, deviation in viscosity, deviation in refractive index, deviation in ultrasonic velocity, degree of inter-molecular attraction, adiabatic compressibility deviation and change of inter-molecular free length were fitted to a Redlich-Kister equation of the type

$$Y^E = x_1 x_2 \sum_{i=0}^{n} A_i \left(x_2 - x_1\right)^i$$

Where Y refers to V^E, $\Delta\eta$, Δn ΔZ, Δu, $\Delta\beta$, ΔL and n is the degree of polynomial.

Coefficients of A_i are obtained by fitting equation to experimental results using least square regression method and the results are tabulated in the below tables.

Table 1 Excess values of interaction parameters - Propane-1-ol + CCL_4 at 308K

Propane-1-ol + CCL_4	Excess adiabatic ($\Delta\beta$) x 10^{-6} m^2/N	Excess free length (ΔL) x 10^{-9} m	Excess velocity (Δu) m/s	Excess viscosity ($\Delta\eta$) cP	Excess Relaxation time x 10^{-10}	Excess molar volume (V^E) m^3/mol x 10^{-13}
1%	-4.0600	1.35	-23	-0.1272	-1.84	1.64
3%	-3.8734	1.70	-64	-0.1366	-8.69	-1.96
5%	6.0519	4.96	-79	-0.14	-1.19	-2.24
7%	8.7549	2.64	-44	-0.1034	-1.15	1.54
9%	4.9693	2.17	-25	-0.0368	-2.83	-9.55

Table 2 Excess values of interaction parameters - Propane-1-ol + CCL_4 at 313K

Propane-1-ol + CCL_4	Excess adiabatic (Δβ) x 10^{-6} m^2/N	Excess free length (ΔL) x 10^{-9} m	Excess velocity (Δu) m/s	Excess viscosity (Δη) cP	Excess Relaxation time x 10^{-10}	Excess molar volume (V^E) m^3/mol x 10^{-13}
1%	1.77386	2.19604	-38	-0.1344	-1.6200	3.8766
3%	-5.2947	1.22616	-50	-0.2112	-2.2779	2.5208
5%	3.68824	4.24504	-67	-0.138	-1.4663	-2.0239
7%	4.52	3.59248	-52	-0.1058	-1.0402	-7.7742
9%	1.9281	2.12506	-24	-0.0736	-7.3388	4.1212

Table 3 Excess values of interaction parameters - Propane-1-ol + CCL_4 at 318K

Propane-1-ol + CCL_4	Excess adiabatic (Δβ) x 10^{-11} m^2/N	Excess free length (ΔL) x 10^{-9} m	Excess velocity (Δu) m/s	Excess viscosity (Δη) cP	Excess Relaxation time x 10^{-10}	Excess molar volume (V^E) m^3/mol x 10^{-13}
1%	1.6982	2.2290	-38.5	-0.1293	-1.5660	4.9346
3%	-3.4763	1.9964	-62.5	-0.2099	-2.0080	2.5120
5%	4.2958	4.5350	-70.5	-0.1755	-1.8723	1.5796
7%	5.2501	3.8588	-54.5	-0.1341	-1.3467	2.8548
9%	3.8577	1.9005	-21.5	-0.0667	-7.2174	3.7502

Table 4 Excess values of interaction parameters - Propane-1-ol + CCL_4 at 323K

Propane-1-ol + CCL_4	Excess adiabatic (Δβ) x 10^{-11} m^2/N	Excess free length (ΔL) x 10^{-9} m	Excess velocity (Δu) m/s	Excess viscosity (Δη) cP	Excess Relaxation time x 10^{-10}	Excess molar volume (V^E) m^3/mol x 10^{-13}
1%	2.3982	2.51765	-42.6	-0.1029	-1.1519	3.6050
3%	-3.40505	2.10224	-62.8	-0.1647	-1.4654	1.9688
5%	3.30126	4.30511	-66	-0.1235	-1.3389	-7.0635
7%	6.41695	4.18551	-56.2	-0.1163	-1.1113	2.9517
9%	5.66169	2.32995	-24.4	-0.0471	-4.3348	1.5775

Table 5 Excess values of interaction parameters - Propane-1-ol + CCL_4 at 328K

Propane-1-ol + CCL_4	Excess adiabatic (Δβ) x 10^{-11} m^2/N	Excess free length (ΔL) x 10^{-9} m	Excess velocity (Δu) m/s	Excess viscosity (Δη) cP	Excess Relaxation time x 10^{-10}	Excess molar volume (V^E) m^3/mol x 10^{-13}
1%	4.4113	1.77698	138.6	-0.1982	-2.8782	3.4641
3%	-4.5200	1.7652	442.8	-0.2326	-2.6416	4.6954
5%	4.2548	4.5671	764	-0.194	-2.3362	3.8846
7%	9.6183	4.9697	1101.2	-0.1424	-1.3984	3.4160
9%	3.3387	1.7776	1475.4	-0.0718	-9.0295	5.1016

Least Square Regression Method

It is a statistical technique to determine the line of best fit for a model. The least square method is specified by an equation with certain parameters on observed data. This method is extensively used in regression analysis and estimation.

General equation of an n[th] degree polynomial is given by

$$y = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + ...a_n x^n$$

where 'y' represents the observed or experimental value corresponding to x_i

The normal equations are

$$\begin{bmatrix} \sum Y = nA_0 + A_1 \sum X + A_2 \sum X^2 + ... + A_n \sum X^n \\ \sum XY = A_0 \sum X + A_1 \sum X^2 + A_2 \sum X^3 + ... + A_n \sum X^{n+1} \\ \sum X^2 Y = A_0 \sum X^2 + A_1 \sum X^3 + A_2 \sum X^4 + ... + A_n \sum X^{n+2} \\ \vdots \\ \sum X^n Y = A_0 \sum X^{n+1} + A_1 \sum X^{n+2} + A_2 \sum X^{n+3} + ... + A_n \sum X^{2n} \end{bmatrix}$$

Substituting these equations in matrix form shows an interesting pattern in the coefficient matrix.

$$\begin{bmatrix} n & \sum X_i & \sum X_i^2 & \sum X_i^3 \dots & \sum X_i^n \\ \sum X_i & \sum X_i^2 & \sum X_i^3 & \sum X_i^4 \dots & \sum X_i^{n+1} \\ \sum X_i^2 & \sum X_i^3 & \sum X_i^4 & \sum X_i^5 \dots & \sum X_i^{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum X_i^n & \sum X_i^{n+1} & \sum X_i^{n+2} & \sum X_i^{n+3} \dots & \sum X_i^{2n} \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \vdots \\ A_n \end{bmatrix} = \begin{bmatrix} \sum Y_i \\ \sum X_i Y_i \\ \sum X_i^2 Y_i \\ \vdots \\ \sum X_i^n Y_i \end{bmatrix}$$

$$AX = Y$$

where A is called the coefficient matrix, X and Y are called column vectors.

$$A = \begin{bmatrix} n & \sum X_i & \sum X_i^2 & \sum X_i^3 \dots & \sum X_i^n \\ \sum X_i & \sum X_i^2 & \sum X_i^3 & \sum X_i^4 \dots & \sum X_i^{n+1} \\ \sum X_i^2 & \sum X_i^3 & \sum X_i^4 & \sum X_i^5 \dots & \sum X_i^{n+2} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ \sum X_i^n & \sum X_i^{n+1} & \sum X_i^{n+2} & \sum X_i^{n+3} \dots & \sum X_i^{2n} \end{bmatrix},$$

$$X = \begin{bmatrix} A_0 \\ A_1 \\ A_2 \\ \vdots \\ A_n \end{bmatrix} \quad \text{and} \quad Y = \begin{bmatrix} \sum Y_i \\ \sum X_i Y_i \\ \sum X_i^2 Y_i \\ \vdots \\ \sum X_i^n Y_i \end{bmatrix}.$$

This matrix equation can be solved numerically, or can be inverted directly if it is well formed, to yield the solution vector

$$X = A^{-1}Y$$

In the present study, for Propane-1-ol and CCL_4, an attempt is made to fit the second polynomial equation and it given by

$$y = a_0 + a_1 x + a_2 x^2$$

Applying Redlich Kister equation,

$$Y^E = x_1 x_2 \sum_{i=0}^{n} A_i \left(x_2 - x_1\right)^i$$

$$Y^E = x_1 x_2 \left(A_0 X^0 + A_1 X^1 + A_2 X^2\right)$$

where $X = (x_2 - x_1)$ are coefficients which are estimated by using method of Least square regression method x_1 and x_2 are mole fraction and Y^E denotes the deviation values of adiabatic compressibility (Δβ), velocity(ΔU), viscosity (Δη), excess molar volume(ΔV^E), free length(ΔL), free volume(ΔV) etc…

For example, for Propane=1-ol + CCL_4 at 308K, the velocity deviation values are calculated by using

$$\Delta u = u - (x_1 u_1 + x_2 u_2)$$

Here, and x_2 = 0.1, so that

$$\left(1122 - (0.9 * 1174 + 0.1 * 884)\right) = -23$$

Similar procedure is followed for calculating remaining values.

By applying all the values in Redlich-Kister polynomial equation, we get

$$-235 = (5)A_0 + (0)A_1 + (1.6)\,A_2$$

$$-6.4 = (0)A_0 + (1.6)A_1 + (0)A_2$$

$$-48 = (1.6)A_0 + (0)A_1 + (0.8704)A_2$$

Substituting these equations in matrix form gives an interesting pattern in the coefficient matrix.

$$\begin{bmatrix} 5 & 0 & 1.6 \\ 0 & 1.6 & 0 \\ 1.6 & 0 & 0.8704 \end{bmatrix} \begin{bmatrix} A_0 \\ A_1 \\ A_2 \end{bmatrix} = \begin{bmatrix} -235 \\ -6.4 \\ -48 \end{bmatrix}$$

This matrix equation can be solved numerically, or can be inverted directly if it is well formed, to yield the solution vector

$$X = A^{-1}Y$$

Using MatLab software, we get the solution as mentioned below,

Redlich-Kister coefficients $\begin{pmatrix} -71.2857 \\ -4 \\ 75.8929 \end{pmatrix}$ obtained for different temperatures are listed in the below tables.

Table 6 Redlich-Kister coefficients @308K

Function	a_0	a_1	a_2	σ
ΔU	-71.2857	-4.000	75.8929	0.00009
Δη	-0.1362	-0.0535	0.0857	0.00008
Δρ	16.8571	-6.000	3.5714	0.00018
Δβ	0.1523	-0.3875	0.0004	0.53886
ΔL	0.3583	-0.0638	-0.3198	0.90496
ΔV	-0.0302	0.0812	0.1655	0.08046
Δt	-0.1089	-0.0712	0.0071	0.376986

Table 7 Redlich-Kister coefficients @313K

Function	a_0	a_1	a_2	σ
ΔU	-62.2	-6.5000	50.00	0.00000
Δη	-0.1579	-0.0568	0.079	0.00007
Δρ	20.3571	-4.0000	-2.678	0.00018
Δβ	-0.0002	-0.0010	0.0017	0.00018
ΔL	0.3344	-0.0556	-0.2083	0.94661

ΔV	-0.0772	-0.1042	0.5055	0.29896
Δt	-0.1648	-0.0753	0.0689	0.50470

Table 8 Redlich-Kister coefficients @318K

Function	a_0	a_1	a_2	σ
ΔU	-69.2143	-10.5	61.6071	0.00009
Δη	-0.1864	-0.0503	0.1353	0.00001
Δρ	20.2714	-4.5	-1.7857	0.00008
Δβ	0.2218	-0.3261	0.0333	0.82177
ΔL	0.3856	-0.0301	-0.2976	1.02660
ΔV	0.2244	-0.1714	-0.0017	0.79145
Δt	-0.1864	-0.0587	0.1127	0.53151

Table 9 Redlich-Kister coefficients @323K

Function	a_0	a_1	a_2	σ
ΔU	-67.1143	-10.75	52.2321	0.00009
Δη	-0.1435	-0.04	0.1018	0.00008
Δρ	1.5571	-1.5402	-0.0031	0.54961
Δβ	0.1945	-0.4087	0.2904	1.01610
ΔL	0.3831	-0.0427	-0.2323	1.09164
ΔV	0.1487	-0.0854	-0.0403	0.48013
Δt	-0.1398	-0.0448	0.093	0.38905

Table 10 Redlich-Kister coefficients @328K

Function	a_0	a_1	a_2	σ
ΔU	762.1143	-833	69.6429	0.000099
Δη	-0.1997	-0.0857	0.0996	0.000099
Δρ	23.7857	-5.25	-4.0179	0.000099
Δβ	0.3491	-0.4983	-0.27	0.928691893
ΔL	0.4223	-0.0801	-0.3911	1.050576819
ΔV	0.3934	-0.0499	0.0558	1.454009532
Δt	-0.2196	-0.1298	0.0513	0.7183639

CONCLUSION

The excess thermo-acoustical parameters are defined as the difference between the experimental values and ideal mixture values. They give a measure of the non-ideality of the system as a consequence of associative or of other interactions. The observed negative and positive deviation parameters are discussed in the light of inter-molecular interactions present in these liquid mixtures. The positive values of V^E, Δu, Δη, Δρ, Δβ, ΔL and ΔV at different temperature 308k, 313k, 318k, 323k and 328k have been calculated which indicate the presence of strong molecular interaction. Negative values of V^E, Δu, Δη, Δρ, Δβ, ΔL and ΔV at different temperature 308k, 313k, 318k, 323k and 328k are estimated which indicate the existence of weak interaction. Thus the mathematical polynomial equation given by Redlich- Kister is used to analyse and discuss in terms of polymer-solvent interactions and it finds whether the nature of interaction between the molecules is strong or weak. The results are interpreted in terms of molecular interactions occurring in the solution.

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COMPUTATION OF NEW DEGREE -BASED TOPOLOGICAL INDICES OF TRIANGULANES

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ABSTRACT:
Let G be a connected graph constructed from pairwise disjoint connected graphs $G_1, \ldots, G_k$ by selecting a vertex of G_1, a vertex of G_2, and identifying these two vertices. Then continue this manner recursively. In this paper, we calculated the Harmonic Index, Augmented Zagreb Index, Geometric-arithmetic Index, Randic connectivity index, Zagerb indices of Triangulane.

Keywords: Topological indices, Molecular graph, Triangulane

INTRODUCTION:
A molecular graph is a simple graph such that its vertices correspond to the atoms and the edge to the bonds of a molecule. Let $G = (V, E)$ be a finite, connected, simple graph. We denote the degree of a vertex v in G by d_v. A topological index of G is a real number related to G. It does not depend on the labelling or pictorial representation of a graph. [1] The wiener index W (G) is the first distance based topological index defined as $w(G) = \sum_{u,v \in (G)} d(u,v) = \frac{1}{2} \sum_{u,v \in V(G)} d(u,v)$ with the summation runs over all pairs of vertices of G. [2, 3]A topological index of a chemical compound is an integer, derived following a certain rule, which can be used to characterize the chemical compound and predict certain physiochemical properties like boiling point, molecular weight, density, refractive index, and so forth. The topological indices and graph invariants based on distance between vertices of a

graph widely used for characterizing molecular graphs, establishing relationships between structure and properties of molecules , predicting biological activity of chemical compounds, and making their chemical applications. The wiener index is one of the most used topological indices with high correlation with many physical and chemical indices of molecular compounds. [4] Recently in a new vertex –degree –based molecular structure descriptor was put forward, the Sombor index, is defined as

$$SO(G) = \sum_{u,v\, \in E(G)} \sqrt{d_u^2 + d_v^2}.$$

[5] Cruz, Gutman and Rada in characterized the graphs extremal with respect to this index over the chemical graphs, chemical trees and hexagon systems (see [6]). In [7], the **chemical**

importance of the Sombor index has investigated and it is shown that this index is useful in predicting physicochemical properties with high accuracy compared to some well-established and often used indices. Also a sharp upper bound for the Sombor index among all molecular trees with fixed numbers of vertices has obtained, and those molecular trees achieving the extremal value have been characterized. [8]In some novel lower and upper bounds on the Sombor index of graphs has presented by using some graph parameters, especially, maximum and minimum degree. Moreover, several relations on Sombor index with the first and second Zagreb indices of graphs were obtained. [9]The mathematical relations between the Sombor index and some other well-known degree-based descriptors investigated .

Topological indices:

In this paper we calculated Harmonic Index, Augmented Zagreb Index, Geometric-arithmetic Index, Randic connectivity index, Zagerb indices of Triangulane.

Harmonic Index

In the 1980s, Siemion Fajtlowicz created a computer program for automatic generation of conjectures in graph theory. [10]Then he examined the possible relations between countless graph invariants, among which there was a vertex-degree-based quantity

$$H(G) = \sum_{u,v\, \in E(G)} \frac{2}{d_u(G) + d_v(G)}$$

With a single exception [11] H(G) did not attract any-body's attention, especially not of chemists. [12,13]Only in 2012, Zhang re-introduced this quantity, and called it "harmonic index". His works were followed by the recent paper .[14] No chemical applications of the harmonic index were reported so far, but, knowing the present situation in mathematical chemistry, such researchers are very much to be expected.

Augmented Zagreb Index

Motivated by the success of the ABC index,[15] Furtula et al. put forward its modified version, that they somewhat inadequately named “augmented Zagreb index”. It is defined as

$$AZI(G) = \sum_{u,v \in E(G)} \left(\frac{d_u(G).d_v(G)}{d_u(G) + d_v(G) - 2} \right)^3$$

Geometric-arithmetic Index

Another recently conceived vertex-degree-based topological index utilizes the difference between the geometric and arithmetic means, and is defined as

$$GA(G) = \sum_{u,v \in E(G)} \frac{\sqrt{d_u(G).d_v(G)}}{\frac{1}{2}[d_u(G) + d_v(G)]}$$

Where, Where, $\sqrt{d_u(G).d_v(G)}$ and $\frac{1}{2}[d_u(G) + d_v(G)]$ are the geometric and arithmetic means respectively, of the degrees of the end-vertices of an edge. Recall that the former is always less than or equal to the later. [16]The index was invented by Vukičević and Furtula and was named “geometric-arithmetic index”.

Soon after the GA index was defined by using the above formula. The idea was replace in the vertex degrees by some other vertex property. By this the second, third, ..., sixth “geometric-arithmetic” indices were constructed, whose chemical relevance is highly doubtful; [17]for details see Reference, the reviews in References [18], [19].This index is referred as first geometric arithmetic index.

Randic connectivity index

[20,21] Historically, the first vertex- degree - based structure descriptors were the graph invariants that nowadays are called Zagreb indices. However, initially these were intended to be used for a completely different purpose and these were included among topological indices much later.[22] The first genuine degree- based topological index was put forward in 1975 by Milan Randic in his seminal paper “On characterization of molecular branching”. His index was defined as

$$R = R\,(G) = \sum_{u,v \in E(G)} \frac{1}{\sqrt{d_u.d_v}}$$

Randic himself named it “ branching index”, [23,24]but soon it was re-named to “ Connectivity index”. Nowadays, most authors refer to it as to the “ Randic index. The suitability of the Randic index for drug design was immediately recognized, and eventually the index was used for this purpose on countless occasion.

Zagerb indices

Analyzing the structure-dependency of total π-electron energy an approximate formula was obtained in which terms of the form

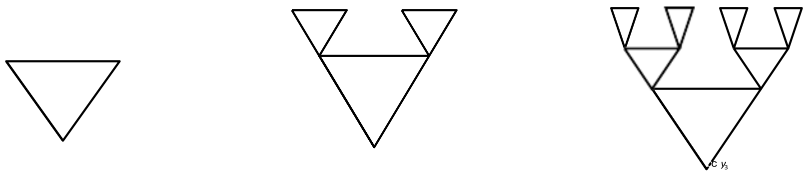
$$M_1\,(G) = \sum_{u,v\,\in E(G)} (d_u +\, d_v)$$

$$M_2\,(G) = \sum_{u,v\,\in E(G)} (d_u . d_v)$$

occured. It was immediately recognized that these terms increase with the increasing extent of branching of the carbon-atom skeleton. i.e., that these provide quantitative measures of molecular branching. Ten years later, in a review article,[25] Balaban et al. included M1 and M2 among topological indices and named them “Zagreb group indices”. The name “Zagreb group index “ was soon abbreviated to “ Zagreb index”, and nowadays $M_1\,(G)$ is referred as the “first Zagreb index”, and $M_2\,(G)$ as the “ Second Zagreb index”.

Triangulane:

[26]We intend to derive the some topological indices of the triangulane T_k defined pictorially in . We define T_k recursively in a manner that will be useful in our approach. First we define recursively an auxiliary family of triangulanes G_k ($k \geq 1$). Let G_1 be a triangle and denote one of its vertices by y_1. We define G_k ($k \geq 2$) as the circuit of the graphs G_{k-1}, G_{k-1}, and K_1 and denote by y_k the vertex where K_1 has been placed. The graphs G_1, G_2 and G_3 are shown in



G_1 G_2 G_3

Figure 1. Graphs G_1, G_2 and G_3

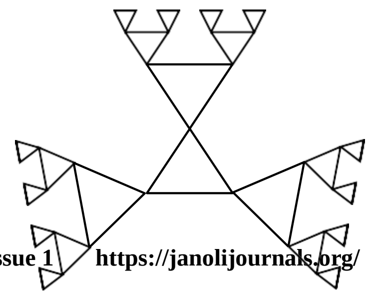


Figure 2. Graphs T_3

Theorem : 1

For the graph T_k (see T_3 in figure 2), we have

$$H(G) = [3+9(2^{k-1})]\frac{1}{4}+3(2^{k-1})\frac{1}{2}+3(2^k)\frac{1}{3}$$

$$\boldsymbol{AZI(G) = 8[[3+9(2^{k-1}-1)]+3(2^{k-1})+3(2^k)]}$$

$$GA(G) = [3+9(2^{k-1}-1)]+3(2^{k-1})+3(2^k)\frac{2\sqrt{2}}{3}$$

$$R(G) = [3+9(2^{k-1}-1)]\frac{1}{4}+3(2^{k-1})\frac{1}{2}+3(2^k)\frac{1}{2\sqrt{2}}$$

$$M_1(G) = 72(2^{k-1}-1)+12(2^{k-1})+18(2^k)+24$$

$$M_2(G) = 144(2^{k-1}-1)+12(2^{k-1})+24(2^k)+48$$

Proof: Since creating such a graph is recursive, then there are $[\boldsymbol{3+9(2^{k-1}-1)}]$ edges with end points of degree 4. Also there are $3(2^k)$ edges with endpoints of degree 4 and 2, and there are $3(2^{k-1})$ edges with endpoints of 2.

Harmonic Index

$$H(G) = \sum_{u,v\in E(G)}\frac{2}{d_u(G)+d_v(G)}$$

$$= \sum_{u,v\, E_1(G)}\frac{2}{d_u(G)+d_v(G)}+\sum_{u,v\, E_2(G)}\frac{2}{d_u(G)+d_v(G)}+\sum_{u,v\, E_3(G)}\frac{2}{d_u(G)+d_v(G)}$$

$$= [3+9(2^{k-1}-1)]\frac{2}{4+4}+3(2^{k-1})\frac{2}{2+2}+3(2^k)\frac{2}{4+2}$$

$$= [3+9(2^{k-1}-1)]\frac{1}{4}+3(2^{k-1})\frac{1}{2}+3(2^k)\frac{1}{3}$$

Augmented Zagreb Index

$$AZI(G) = \sum_{u,v\,\in E(G)} \left(\frac{d_u(G).\,d_v(G)}{d_u(G)+d_v(G)-2}\right)^3$$

$$AZI(G) = \sum_{u,v\,\in E_1(G)} \left(\frac{d_u(G).\,d_v(G)}{d_u(G)+d_v(G)-2}\right)^3 + \sum_{u,v\,\in E_2(G)} \left(\frac{d_u(G).\,d_v(G)}{d_u(G)+d_v(G)-2}\right)^3$$

$$+ \sum_{u,v\,\in E_3(G)} \left(\frac{d_u(G).\,d_v(G)}{d_u(G)+d_v(G)-2}\right)^3$$

$$= \left[3+9\left(2^{k-1}-1\right)\right]\left(\frac{4\times4}{4+4-2}\right)^3 + 3(2^{k-1})\left(\frac{2\times2}{2+2-2}\right)^3 + 3(2^k)\left(\frac{4\times2}{4+2-2}\right)^3$$

$$= \left[\mathbf{3}+\ \mathbf{9}\left(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}}-\mathbf{1}\right)\right]\left(\frac{\mathbf{16}}{\mathbf{6}}\right)^{\mathbf{3}} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}})\left(\frac{\mathbf{4}}{\mathbf{2}}\right)^{\mathbf{3}} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}})\left(\frac{\mathbf{8}}{\mathbf{4}}\right)^{\mathbf{3}}$$

$$= \left[\mathbf{3}+\mathbf{9}\left(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}}-\mathbf{1}\right)\right](\mathbf{2.67})^{\mathbf{3}} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}})\,(\mathbf{2})^{\mathbf{3}} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}})(\mathbf{2})^{\mathbf{3}}$$

$$= \left[\mathbf{3}+\mathbf{9}\left(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}}-\mathbf{1}\right)\right]\mathbf{8} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}})\,\mathbf{8} + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}})\mathbf{8}$$

$$= \mathbf{8}[\left[\mathbf{3}+\mathbf{9}\left(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}}-\mathbf{1}\right)\right] + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}-\mathbf{1}}) + \mathbf{3}(\mathbf{2}^{\boldsymbol{k}})]$$

Geometric-arithmetic Index

$$GA(G) = \sum_{u,v\,\in E(G)} \frac{\sqrt{d_u(G).\,d_v(G)}}{\frac{1}{2}[d_u(G)+d_v(G)]}$$

$$= \sum_{u,v\,\in E_1(G)} \frac{\sqrt{d_u(G).\,d_v(G)}}{\frac{1}{2}[d_u(G)+d_v(G)]} + \sum_{u,v\,\in E_2(G)} \frac{\sqrt{d_u(G).\,d_v(G)}}{\frac{1}{2}[d_u(G)+d_v(G)]} + \sum_{u,v\,\in E_3(G)} \frac{\sqrt{d_u(G).\,d_v(G)}}{\frac{1}{2}[d_u(G)+d_v(G)]}$$

$$= \left[3+9\left(2^{k-1}-1\right)\right]\frac{\sqrt{4\times4}}{\frac{1}{2}[4+4]} + 3(2^{k-1})\frac{\sqrt{2\times2}}{\frac{1}{2}[2+2]} + 3(2^k)\frac{\sqrt{4\times2}}{\frac{1}{2}[4+2]}$$

$$= \left[3+9\left(2^{k-1}-1\right)\right][\tfrac{4}{4}] + 3(2^{k-1})[\tfrac{2}{2}] + 3(2^k)\frac{2\sqrt{2}}{3}$$

$$= \left[3+9\left(2^{k-1}-1\right)\right] + 3(2^{k-1}) + 3(2^k)\frac{2\sqrt{2}}{3}$$

Randic connectivity index

$$R = R\,(G) = \sum_{u,v\,\in E(G)} \frac{1}{\sqrt{d_u.\,d_v}}$$

$$R = R\,(G) = \sum_{u,v\,\in E_1(G)} \frac{1}{\sqrt{d_u.d_v}} + \sum_{u,v\,\in E_2(G)} \frac{1}{\sqrt{d_u.d_v}} + \sum_{u,v\,\in E_3(G)} \frac{1}{\sqrt{d_u.d_v}}$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right]\frac{1}{\sqrt{4\times 4}} + 3(2^{k-1})\frac{1}{\sqrt{2\times 2}} + 3(2^k)\frac{1}{\sqrt{4\times 2}}$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right]\frac{1}{\sqrt{16}} + 3(2^{k-1})\frac{1}{\sqrt{4}} + 3(2^k)\frac{1}{\sqrt{8}}$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right]\frac{1}{4} + 3(2^{k-1})\frac{1}{2} + 3(2^k)\frac{1}{2\sqrt{2}}$$

Zagerb indices:

$$M_1\,(G) = \sum_{u,v\,\in E(G)} (d_u + d_v)$$

$$= \sum_{u,v\,\in E_1(G)} (d_u + d_v) + \sum_{u,v\,\in E_2(G)} (d_u + d_v) + \sum_{u,v\,\in E_3(G)} (d_u + d_v)$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right](4 + 4) + 3(2^{k-1})\,(2 + 2) + 3(2^k)(4 + 2)$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right]8 + 3(2^{k-1})4 + 3\left(2^k\right)6$$

$$= 72\left(2^{k-1} - 1\right) + 12(2^{k-1}) + 18\left(2^k\right) + 24$$

$$M_2\,(G) = \textstyle\sum_{u,v\,\in E(G)} (d_u.d_v)$$

$$= \textstyle\sum_{u,v\,\in E_1(G)} (4\times 4) + \sum_{u,v\,\in E_2(G)} (2\times 2) + \sum_{u,v\,\in E_3(G)} (4\times 2)$$

$$= \left[3 + 9\left(2^{k-1} - 1\right)\right]16 + 3(2^{k-1})\,4 + 3(2^k)8$$

$$= 144\left(2^{k-1} - 1\right) + 12(2^{k-1}) + 24\left(2^k\right) + 48$$

CONCLUSION

Topological indices are used for example in the development of quantitative structure – activity relationships (QSARs) in which the biological activity or other properties of molecules are correlated with their chemical structure. In this paper, a generalized formula for Harmonic index, Augmented Zagreb Index, Geometric-arithmetic Index, Randic connectivity index, Zagerb indices of Triangulane has been calculated without using the computer.

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EXAMINATION OF PANDEMIC COVID-19 MATTER TO EVALUATE INDIA'S AWAKENING

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Abstract: This paper's primary goal was to evaluate Indian human understanding of the COVID-19 pandemic, which is currently posing an imminent danger to worldwide public health due to the rise and dissemination of the “2019 novel coronaviruses (2019-nCoV)”, also known as the “grave acute respiratory syndrome coronavirus 2 (SARS-CoV-2)”. The virus was first discovered in bats and spread to humans in Wuhan, Hubei province, China in December 2019 via as-yet-unidentified intermediate species to get their opinions, a survey was created, and the relevant analytical hypothesis investigation was run to understand the results. For adults (male and female), as well as teens, not a noticeable distinction was seen. For consciousness, nearly the same viewpoint was noted with a Kruskal-Wallis Test (H) score of 1.5619. According to actual considerations, all teens and adults with a decent understanding, regardless of gender, have the identical capacity and ability to deal with the challenges posed by the COVID-19 epidemic.

Keywords: Awareness, Covid 2019, pandemic, disease, teenagers, adults, precautions

INTRODUCTION: From the beginning in Wuhan City, Hubei Province, China, the 2019 newly identified corona virus (2019-nCoV), also known as the stringent acute respiratory syndrome-related corona virus 2 (SARS-CoV-2), has traveled quickly across various parts of the globe[1]. Up to June 29, 2020, there have been documented 10,249377 instances of COVID-19, 504,466 fatalities, and 5,556,634 recoveries [2]. To far, India has recorded 16475 death cases, 321723 recovering cases, and 548318 verified cases. An inflammatory condition known as coronavirus syndrome (COVID-19) is brought on by a recently identified coronavirus. The majority of COVID-19 virus infections result in mild to severe breathing disorders and are treated normally. Elderly people or those with a medical history of cancer, heart disease, diabetes, or persistent asthma are more prone to suffer from serious illness. The best way to prevent and delay infection is to become fully informed about the COVID-19 virus, the disease it causes, and the way it spreads. To avoid becoming sick, keep your hands clean and avoid touching your face. You can also use an alcohol-based face massage to help prevent infections in other people. Thoracic hygiene is vital since the COVID-19 virus is mostly communicated by drops of spit or fluid from one's nostrils when the infected individual wheezes or coughs (for example, by sneezing into a bent elbow). There are currently no COVID-19-specific vaccinations or therapies available[3]. Warning is always preferable than treatment, as we all know.

MATERIAL AND METHODS

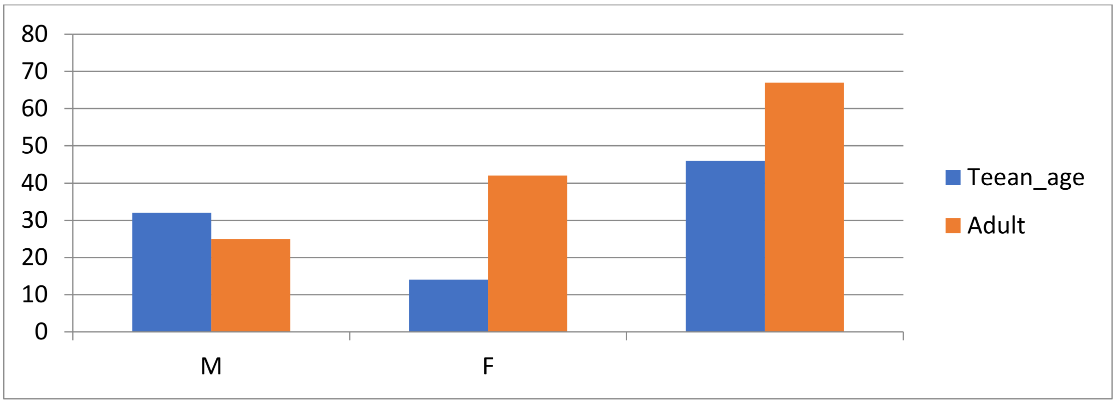
The paper's goal is to evaluate Indian society's knowledge of the COVID-19 epidemic. Students' opinions were gathered via the creation of a survey, and the results were interpreted using the proper method of hypothesis testing. Responses to our web-based poll came from 46 teenagers (32 men and 14 women) and 67 seniors (25 men and 42 women). By region, India is located northern of the tropics between latitudes 8°4' north and 37°6' north and longitudes 68°7' eastern and 97°25' eastern.

- To learn what teens think in order to gauge their level of knowledge on COVID-19.
- To get adult viewpoints in order to gauge knowledge of COVID-19.
- To find out what each gender thinks in order to gauge knowledge of COVID-19.

RESULTS:

Thoughts noticed throughout the current investigation are given using tables to support the data collection. The objective of this study is to conduct suitable statistical analyses on the information to verify the statistical assertion. This theory aids in the interpretation of data and explains the opinions of adults, teens, and learners on the global epidemic sickness COVID-19. For seniors (male and female), as well as teens, little variation was seen. For understanding, nearly the same viewpoint was noted with a Kruskal-Wallis Test (H) value of 1.5619. According to actual considerations, all adolescents and adults with a decent awareness, regardless of gender, have identical capacities and abilities to deal with the challenges posed by the COVID-19 epidemic.

Table No:4 Group Statistics between both teenager and adult



We are able to quickly calculate a total of rankings for every participant using the data supplied about the young age female reaction, senior female reaction, youth age male reaction, and older male reaction:

R_1 = 8 + 18.5 + 18.5 + 18.5 + 38.5 + 58.5 + 75 + 75 + 75 + 87.5 + 107.5 + 107.5 + 107.5 + 107.5 = 903

R_2 = 3.5 + 8 + 8 + 8 + 18.5 + 18.5 + 18.5 + 18.5 + 18.5 + 18.5 + 18.5 + 18.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 58.5 + 58.5 + 58.5 + 58.5 + 58.5 + 58.5 + 75 + 75 + 75 + 75 + 75 + 87.5 + 87.5 + 87.5 + 87.5 + 94.5 + 94.5 + 99.5 + 99.5 + 107.5 + 107.5 + 107.5 = 2270

R_3 = 1 + 3.5 + 3.5 + 8 + 18.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 58.5 + 58.5 + 58.5 + 58.5 + 58.5 + 58.5 + 58.5 + 75 + 75 + 75 + 75 + 75 + 87.5 + 87.5 + 94.5 + 99.5 + 107.5 + 107.5 = 1749.5

R_4 = 3.5 + 18.5 + 18.5 + 18.5 + 18.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 38.5 + 58.5 + 58.5 + 75 + 75 + 75 + 75 + 87.5 + 94.5 + 94.5 + 94.5 + 99.5 + 107.5 + 107.5 + 107.5 = 1518.5

(1) *Parallel and Blank The theories*

Testing is required for the subsequent empty and competing predictions:

Ho: The specimens are drawn from equal-middle groups.

Ha: The numbers from which the specimens are drawn have varying averages.

The test known as Kruskal-Wallis is going to be used to evaluate the aforementioned theories.

(2) *Region of Refusal*

According to the data supplied, there are df = 4 - 1 = 3df = 4−1=3 levels of autonomy and a threshold of importance of α=.05. For such Chi-Square examination, the rejecting area is thus R = \{\chi^2: \chi^2 > 7.815\}R={χ2:\2>7.815}.

(3) *Examine the Statistics*

We can just input the numbers using the Kruskal-Wallis test program to do the

Kruskal-Wallis Test Calculator: The subsequent equation is used to obtain the H statistics: H = (∑T2/n) - 3(N+1) * (12/(N(N+1)) = H = 0.001 * 368813.731 - 342 = 1.5619With N = 113, the H statistic is 1.5619.

(4) *Choosing the null hypothesis*

Since it has been demonstrated that \chi^2 = 1.562 \leq \chi_U^2 = 7.815χ2=1.562≤χU2=7.815, the idea of a null prediction is not rejected.
Using the P-value technique It might be said that the null hypothesis is not refuted since p = 0.6681 \geq.05p=0.6681≥.05 and the p-value of p = 0.6681p=0.6681 support this claim.

(5) *Conclusion*

It is determined that there is no rejection of the null assumption, Ho. Consequently, at the α=.05 significant level, there is little reason to assert that a few of the group's averages are uneven.

CONCLUSIONS

This research is useful in determining the opinions of adult respondents to the consciousness questionnaire about COVID-19, the opinions of teenage learners about COVID-19, and the opinions of both genders regarding COVID-19 attention questionnaires. For elders (male and female), as well as teens, no apparent distinction was seen. For consciousness, nearly the same viewpoint was noted with a Kruskal-Wallis Test (H) value of 1.5619. According to actual considerations, all adolescents and adults with a decent understanding, regardless of gender, have the same capacity and ability to deal with the challenges posed by the COVID-19 epidemic. This could be the result of the finest education efforts, the Indian administration's adoption of safety precautions to halt the pandemic sickness, and PM Modi ji's broadcasting and webcast speeches educating the population about the need to take certain actions and make concessions. We can stop the COVID-19 epidemic if we follow the right safety procedures, wear masks, and keep social distance.

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A Review Based on Hydrogen Fuel Cell`s Hybrid System, their Applications and Energy Management Strategies

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Abstract

Hydrogen fuel cell hybrid systems have emerged as a promising solution for clean and efficientpower generation in transportation, backup power systems, remote power generation, grid and energy storage. This abstract explores their applications and energy management strategies. Hydrogen fuel cell hybrid systems combine hydrogen fuel cells with other energy storage and conversion technologies, such as batteries or supercapacitors, to optimize energy efficiency and address the limitations of standalone fuel cell systems. These hybrid systems offer several advantages, including increased power density, extended range, and improved transient response. In terms of applications, hydrogen fuel cell hybrid systems find utility in various sectors, including transportation, stationary power generation, and portable devices. Inthe transportation sector, they can power electric vehicles (EVs) by supplying electricity to anelectric motor, thereby eliminating the need for conventional fossil fuel engines. Stationary applications include backup power systems for buildings and remote locations, as well as gridsupport and renewable energy integration. Additionally, hydrogen fuel cell hybrid systems canbe integrated into portable devices, such as laptops or drones, providing a clean and reliable power source. Energy management strategies play a crucial role in optimizing the performance and efficiencyof hydrogen fuel cell hybrid systems. These strategies involve intelligent control algorithms that govern the distribution of power between different components, such as fuel cells, batteries, and supercapacitors. The aim is to achieve optimal operation based on factors like power demand, energy availability, and system efficiency. Energy management strategies typically involve real-time monitoring, prediction of power demand, and dynamic allocation of power sources to ensure efficient and reliable operation of the hybrid system. This study emphasizes on the applications of hydrogen fuel cell systems and their benefits in power generation, efficiency and environmental sustainability.

Keywords: Hydrogen fuel cell, Hybrid system, Hybrid vehicles, Energy Management Strategy

INTRODUCTION

The increasing usage of petroleum and gas are aggravating environmental issues, and at this time, energy shortages and ecological protection are receiving considerable attention in many nations. Hydrogen energy and fuel cells are thought of as possible alternatives to attain zero- pollution emissions among the numerous energy sources and technologies to replace fossil fuels. In many nations, the automobile industry is significant, and cars are a need for people togo around on a daily basis. As long as traditional fuel vehicles continue to hold a sizable portionof the market, they will contribute significantly to air pollution and greenhouse gas emissions while being driven. Pollutant and greenhouse gas emissions can be significantly reduced by switching to clean energy sources like electricity and hydrogen for vehicle propulsion.

The fuel cells covered in this article are proton exchange membrane fuel cells (PEMFCs), which produce power using hydrogen as the fuel. The hydrogen's chemical energy is directly transformed into electricity, heat, and water by the PEMFC. The fuel cell struggles with a delayed dynamic response and finding solutions to challenging driving situations. In a fuel cellthat generates electricity, the hydrogen's chemical reaction is frequently slower than the pace at which the load is changing. During driving, the fuel cell's durability will also be impacted by sudden acceleration and deceleration as well as frequent start-stop operations. Due to thesequalities, fuel cells are frequently combined with other energy sources, such as batteries and ultracapacitors, in hybrid energy storage systems for power applications. Fuel cells are also frequently employed in hybrid power systems, which combine them with other energy sources.Reduced hydrogen use, smaller fuel cells, and more cost-effective hybrid power systems are all beneficial. Unmanned aerial vehicles (UAVs) and trams are just two examples of the transportation equipment that frequently uses fuel cell-based hybrid systems. This demonstrates how the importance of hydrogen energy in the transportation sector is growing.

Fuel cell hybrid vehicles typically have batteries or ultracapacitors as auxiliary energy sourcesin addition to using fuel cells as their primary power source. The operating circumstances for cars using the road are extremely complicated. They frequently deal with different emergencies, and the needed power demand will likewise experience significant variations andabrupt shifts. However, if solely fuel cells are employed as the energy source, the life of the fuel cell may be shortened by the output of significant power fluctuations. Consequently, the supplemental energy source's function is essential. Ultracapacitors and batteries can both be useful as auxiliary energy sources. When the load demand for power is strong, batteries can capture extra energy and power the system alongside fuel cells. The ultracapacitor can operate as a timely response in the face of rapid variations in load demand thanks to its features of a fast dynamic response, quick energy recovery, and high specific power. There are currently three basic system architectures for fuel cell hybrid cars. The first kind is a hybrid system made up of batteries and fuel cells. The second is a hybrid system made up of ultracapacitors and fuel cells. A hybrid system made up of fuel cells, batteries, and ultracapacitors is the last type.The design of the power system has been examined and explored for many types of fuel cell hybrid vehicles.

Fuel cell hybrid cars' performance and efficiency are greatly influenced by EMSs. Its primarygoal is

power distribution between various energy sources while achieving two objectives: first, lowering hydrogen use or similar energy consumption, and second, lengthening fuel cell life, which also translates to improving the economy of the hybrid system. These two optimizationobjectives are the main focus of numerous energy management systems. The rule-based technique is the first category of EMSs. To find the fuel cell's operating point with the best efficiency, it is typically necessary to determine the power map of the fuel cell. In accordancewith the state of the power system, it can also modify how much power is distributed betweenthe fuel cell and the energy storage system (battery or ultracapacitor). It does, however, have anumber of drawbacks, including parameters that are impacted by the test operating settings, a lack of flexibility to various operating situations, and subpar control outcomes. Online optimization strategies and offline optimization strategies are two of the most researched types of optimization-based energy management strategies. Among them, the model predictive control (MPC)-based real-time optimal energy management technique has been the subject ofextensive discussion during the past two years. The learning-based energy management strategies fall under the third group. Its core concept is to train the strategy's parameters to achieve optimal control by using vast real-time and historical data sets. Researchers have also recently developed an energy management method based on intelligent vehicle interconnectiontechnology, which is presented in this publication. Common energy management techniques for fuel cell hybrids are categorized Optimizing energy usage and extending the life of fuel cells and other components make up the heart of optimization, regardless of the type of energymanagement technique used.[1]

The following topics are the main subject of this essay. The first step is to list the typical hybridsystem used in fuel cell hybrid cars. With batteries, ultracapacitors, or both batteries and ultracapacitors, the fuel cell can create a hybrid power system. FCHEVs frequently employ these three types of hybrid power systems. The most recent fuel cell hybrid vehicle energy management techniques are then categorized and summarized. hydrogen fuel cell hybrid systems are innovative and promising technologies that combine thebenefits of both hydrogen fuel cells and conventional internal combustion engines or electric motors.[2] This hybrid approach aims to address the limitations of individual power sources while maximizing energy efficiency and reducing environmental impact.[3] A hydrogen fuel cell is an electrochemical device that converts hydrogen and oxygen into electricity, producingonly water vapor as a by-product. Fuel cells offer high energy efficiency and zero tailpipe emissions, making them a clean and sustainable power source.[4] However, fuel cells often face challenges such as limited power density and refuelling infrastructure. To overcome theselimitations, hydrogen fuel cell hybrid systems integrate a fuel cell stack with other power sources.[5] One common configuration is combining the fuel cell with a battery pack or an ultra-capacitor system. This hybridization allows for more efficient energy utilization, as the fuel cell provides steady power output while the battery or ultra-capacitor handles peak powerdemands and regenerative braking.[6]

The hybrid system can be applied to various transportation sectors, including cars, buses, trucks, trains, and ships.[7] For example, in hybrid fuel cell electric vehicles (FCEVs), the fuelcell generates electricity to power the electric motor, and the battery or ultra-capacitor stores excess energy for later use or to provide additional power during acceleration or climbing steepslopes. The benefits of hydrogen fuel cell hybrid systems are numerous. Firstly, they offer extended driving ranges compared to pure electric vehicles by leveraging the high energy density of hydrogen.[8] Secondly, the hybrid configuration addresses the slow response and high cost of fuel cells, as the battery or ultra-capacitor can deliver instantaneous power when needed. Additionally, regenerative braking allows for energy recovery, improving overall system efficiency. Lastly, the hybridization enables a more robust and flexible vehicle design,accommodating diverse driving conditions and optimizing the use of different power sources.[9] Hydrogen fuel cell hybrid systems hold significant potential for reducing greenhouse gas emissions, enhancing energy security, and fostering sustainable transportation.[10] Continuedresearch, development, and investment in infrastructure are crucial to overcome technical challenges, lower costs and establish a comprehensive hydrogen ecosystem to support widespread adoption of these systems.[11]

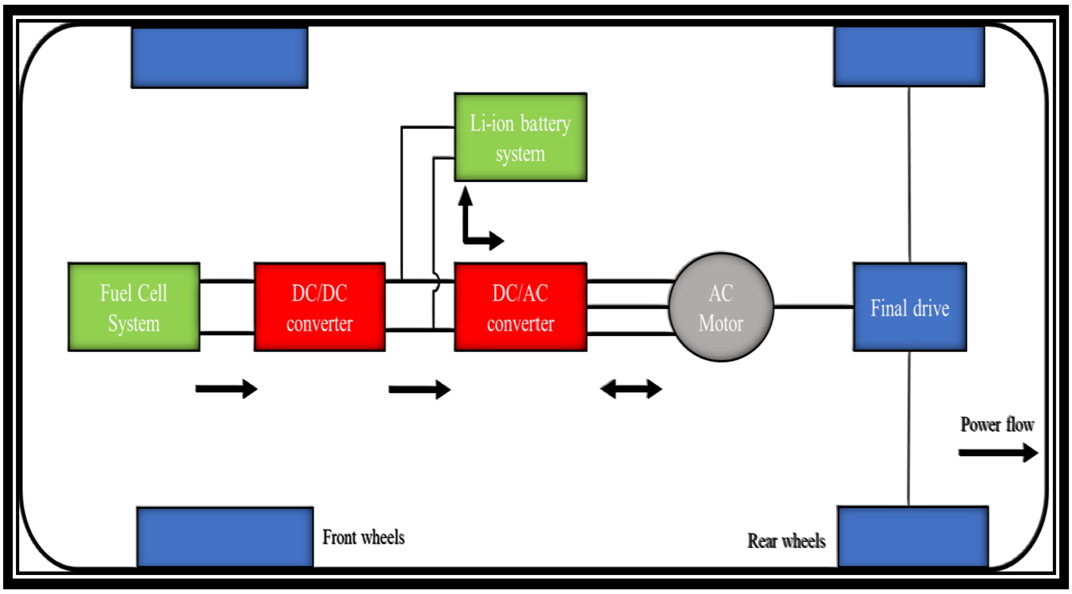
2. VARIOUS HYBRID SYSTEMS

Hydrogen fuel cell hybrid systems are typically designed to combine the benefits of hydrogenfuel cells with other energy storage or generation technologies. Here are some common types of hydrogen fuel cell hybrid systems:

2.1 FC AND BATTERY HYBRID SYSTEM

The most popular topology is a hybrid power source that combines fuel cells and batteries. Battery advantages include high energy density, minimal maintenance requirements, and cheapprice. Battery life cycles typically last 4-6 years. Due to its widespread use in production, thisform of hybridization is the most prevalent topology. Two typical topologies for FC plus battery hybridization exist. The battery is the first and is connected straight to the DC bus. The battery that is attached to the DC bus after the DC/DC converter is also the other. To power the majority of the burden in this system, fuel cells are used as the primary power source. The benefit of this method is that it can recover braking energy. However, compared to FC + UC hybridization, its dynamic reaction is slower.[12]

(i)



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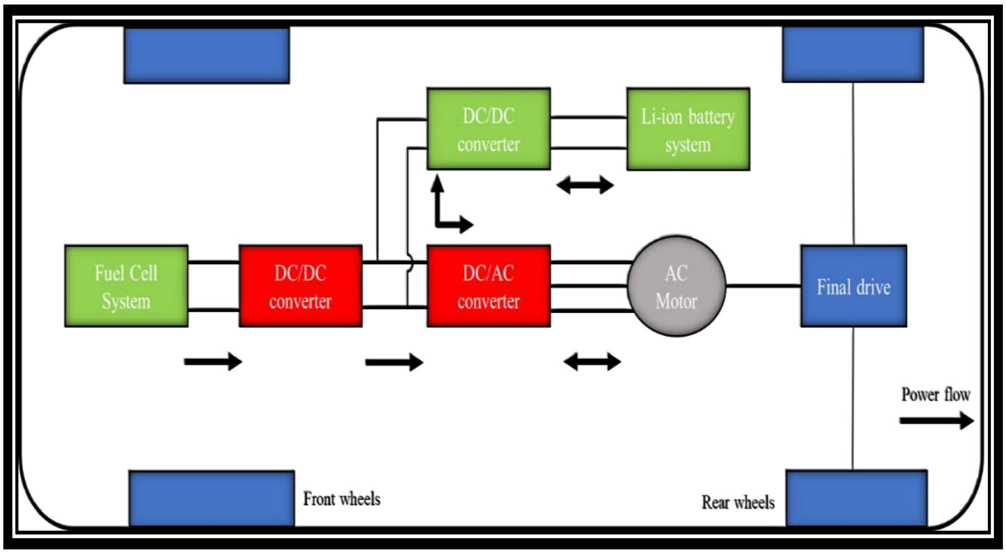
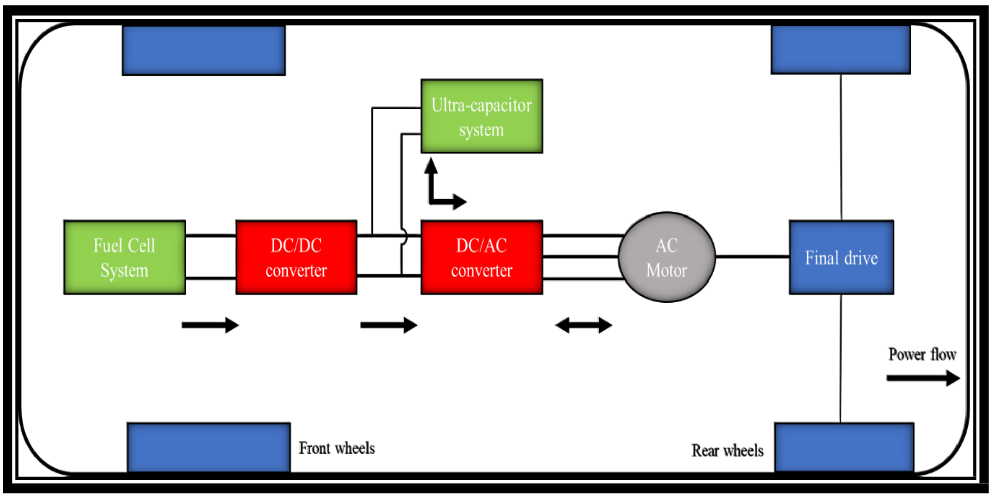


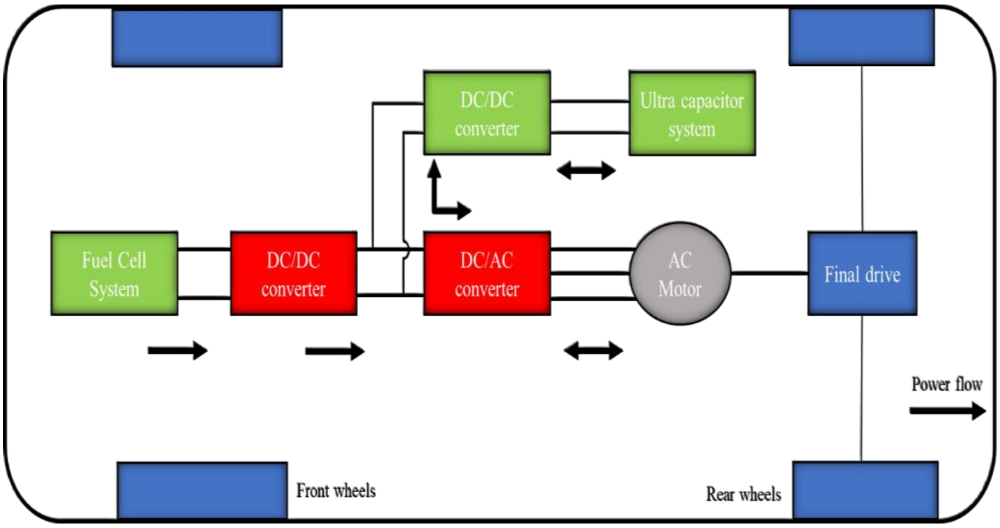
I. FIGURE 1: SCHEMATIC LAYOUT OF FUEL CELL AND BATTERY HYBRID SYSTEM

2.2 FC AND UC HYBRID SYSTEM

Ultracapacitors have the benefits of fast charge and discharge as well as being able to be usedmore frequently in comparison to the drawbacks of batteries, such as low energy density, largesize, and small instantaneous charge and discharge current. Additionally, the lifespan of UC istypically 12 to 20 years. The hybrid system can also be divided into two kinds based on whetherthe ultracapacitor is connected to the DC bus through a DC and DC converter. A completely active topology is typically used because the ultracapacitor's voltage fluctuation is too great. The advantages of this system include greater dynamic response to sudden high-power demand and more effective power recovery. It is less popular than hybrid power systems usingfuel cells and batteries because it also has the drawbacks of high economic cost.[13]

(i)





(ii)

Figure 2: Schematic layout of Fuel cell and Ultracapacitors.

2.3 FULLY FCEV

This system requires no additional energy source. Fuel cells are the only source of energy used by the fused electric vehicles. This system is simple which includes a fuel cell stack, DC/DC converter, an inverter, and an electric generator as shown in Figure 3. It has the qualities of being simple to manage and realize because of its straightforward structure. The majority of frequently used applications are in low-speed vehicles like forklifts, buses, aircraft,trams, and maritime vehicles.[14]

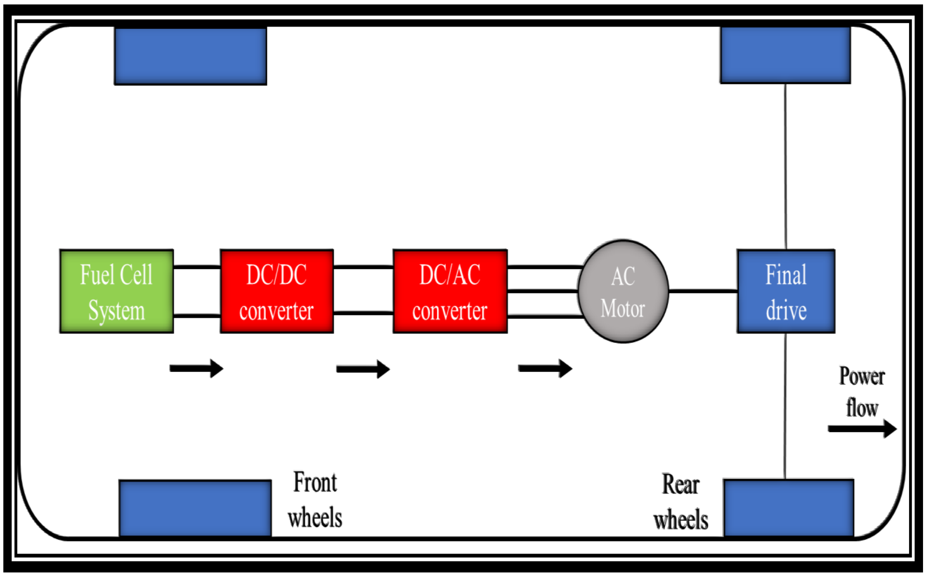


Figure 3: Schematic layout of Fuel cell electric vehicle.

2.4 FC + Battery + UC Hybrid System

The fuel cell, battery, Ultracapacitors hybrid power system's architecture is shown in figure 4. To provide the typical power requirements of the load, the hybrid system continues to rely on fuel cells as itsprimary energy source. In order for batteries and ultracapacitors to function in a variety of conditions, their characteristics are taken into account in their entirety

(i)

(ii)

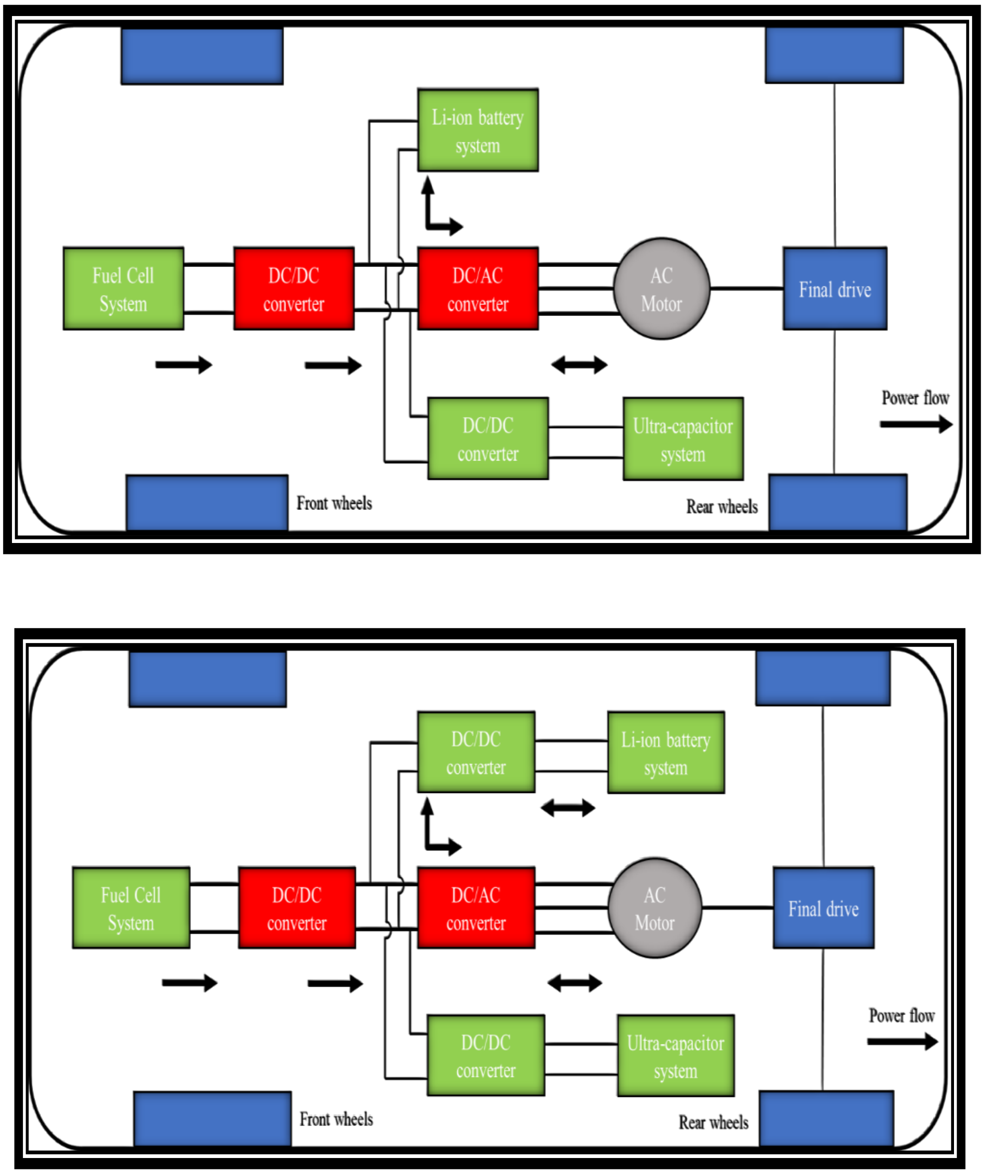


Figure 4: Schematic layout of Fuel cell, battery and Ultracapacitors

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Although they have a tiny energy storage, ultracapacitors have the ability to charge and discharge quickly with high current. When the power needed by the load has significant sudden shifts, ultracapacitors can be used to provide instantaneous power or energy recovery. However, this system's management strategy is challenging because of the hybrid system's intricate structure and the tight coupling between its power sources.[15]

2.5 SUPERCAPACITOR-FUEL CELL HYBRID SYSTEM

Similar to the battery-fuel cell hybrid system, this configuration combines a hydrogen fuel cellwith a supercapacitor.[16] Supercapacitors have higher power density and faster charge/discharge rates compared to batteries, making them suitable for applications that requirequick bursts of power. The supercapacitor assists the fuel cell during high power demands andenergy recovery, improving overall system efficiency.[17]

2.6 COMBUSTION ENGINE-FUEL CELL HYBRID SYSTEM

In this hybrid system, a hydrogen fuel cell is combined with a traditional combustionengine.[18] The fuel cell provides clean and efficient power for normal driving conditions, while the combustion engine can be activated during high-load situations or when additional power is required. This configuration offers the advantages of both technologies, with reducedemissions and increased range compared to a pure combustion engine vehicle.[19]

2.7 SOLAR-FUEL CELL HYBRID SYSTEM

This type of hybrid system combines a hydrogen fuel cell with a solar power generation system.[20] Solar panels generate electricity from sunlight, which can be used directly to powerthe fuel cell or stored in a battery for later use. The fuel cell acts as a backup power source when solar energy is not available or during periods of high-power demand.[21]

2.8 WIND-FUEL CELL HYBRID SYSTEM

Similar to the solar-fuel cell hybrid system, this configuration combines a hydrogen fuel cell with a wind turbine.[22] The wind turbine generates electricity from wind energy, which can be used to power the fuel cell or stored in a battery. The fuel cell serves as a backup power source or provides additional power during periods of low wind speeds.[23]

II. 3.APPLICATION OF HYDROGEN FUEL CELL`S HYBRID SYSTEM

Hybrid systems combining hydrogen fuel cells with other technologies have several potential applications across various industries.[24] Here are some examples:

(i) Transportation: Hydrogen fuel cell hybrid systems can be used in vehicles to provide cleanand efficient power. They offer extended range and faster refueling times compared to pure electric vehicles.[25] These systems can be integrated into cars, buses, trucks, trains, and evenships, providing zero-emission transportation options.[26]

(ii) Backup Power Systems: Fuel cell hybrid systems can be employed as backup power sourcesfor critical infrastructure, such as hospitals, data centres, and telecommunication facilities.[27]These systems can provide reliable and uninterrupted power during outages, ensuring the continuous operation of essential services.[28]

(iii) Remote Power Generation: Hydrogen fuel cell hybrids can be deployed in off-grid or remote locations where access to the electrical grid is limited.[29] These systems can use renewable energy sources, such as solar or wind, to produce hydrogen and then use fuel cells to convert that hydrogen back into electricity when needed.[30] This setup provides a sustainable and reliable power solution for remote communities or industrial sites.[31]

(iv) Portable Power: Fuel cell hybrids can be utilized as portable power sources for various applications, including camping, military operations, and outdoor events.[32] These systems can provide clean and quiet power without the need for traditional fuel combustion, offering a more environmentally friendly alternative to conventional generators.[33]

(v) Grid Energy Storage: Hydrogen fuel cell hybrids can be integrated into energy storage systems for the electrical grid.[34] Excess electricity generated during periods of low demandcan be used to produce hydrogen, which is then stored and later converted back into electricityduring peak demand periods. This setup helps balance the grid, improve energy management,and increase the utilization of renewable energy sources.[35]

(vi) Industrial Applications: Fuel cell hybrid systems can be used in industrial settings, such as manufacturing facilities or warehouses, to provide on-site power generation.[36] These systems can reduce reliance on the grid, lower energy costs, and contribute to the decarbonization of industrial processes.[37]

3. Energy Management Strategies

Current automakers urgently need to create and develop effective energy management systemsto boost the performance of fuel cell hybrids.[38]

The performance of hybrid vehicles is currently being improved through the application of mainstream energy management techniques, both in terms of energy usage and component

durability.[38] Reducing hydrogen use is the major task from the standpoint of energyconsumption.[39] It concentrates on reducing the deterioration of fuel cells, batteries, and ultracapacitors from the standpoint of enhancing component durability.[40] Rule-based energy management strategies, optimization-based energy management strategies, and learning-basedenergy management strategies can be used to categorise common energy management techniques.[41]

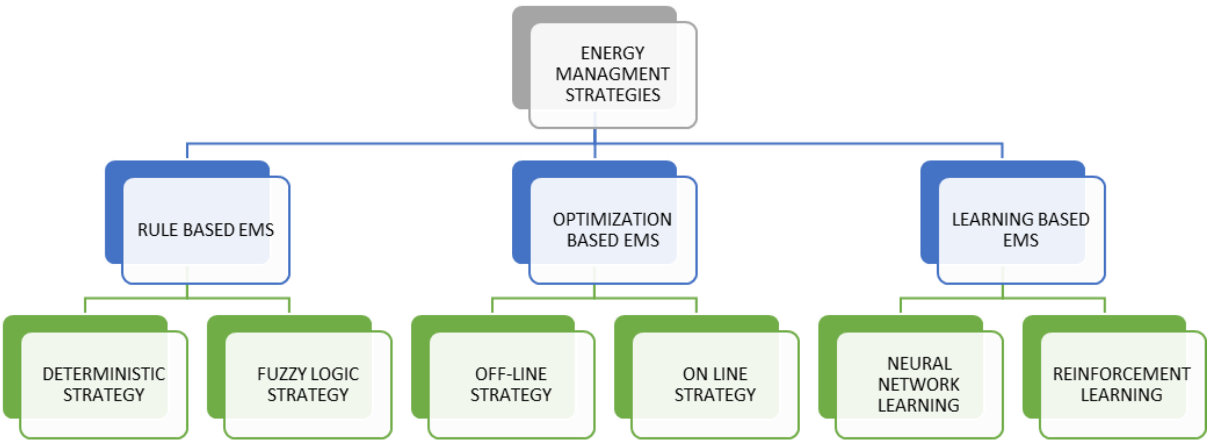

Figure 5: Various energy management strategies.

CONCLUSION

In conclusion hydrogen fuel cell hybrid systems have diverse applications and offer numerous benefits in terms of power generation, efficiency, and environmental sustainability. These hybrid systems combine hydrogen fuel cells with other energy storage and conversion technologies, such as batteries or supercapacitors, to optimize energy efficiency and address the limitations of standalone fuel cell systems. The paper also discusses various energy management strategies that play a crucial role in optimizing the performance and efficiency of hydrogen fuel cell hybrid systems. These strategies involve intelligent control algorithms that govern the distribution of power between different components, such as fuel cells, batteries, and supercapacitors. The aim is to achieve optimal operation based on factors like power demand, energy availability, and systemefficiency.

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Conflicts of Interest

The authors declare no conflict of interest.

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