

NOVEL QUANTUM GRAVITY APPROACH TO EVALUATE THE DIMENSIONALITIES AND THE GEOMETRICAL PROFILES OF THE CHEMICAL REACTIONS

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Abstract

The physical parameters with which the subject of 'Chemical Kinetics' deal are principally the rates and rate constants, the order and the activation energies of chemical reactions.

In this article a novel approach has been made to understand the physics and the dimensionalities (geometrical shapes) of the above said physical parameters by unification of the theory of chemical kinetics and the recently discovered theory of quantum gravity. A new mathematical equation has been developed co-relating the rate constant, the order of the reactions and the activation energies (or activation volume) of the chemical reactions utilizing the physics of formation and the geometries of entropy graviton, mass graviton, volume graviton and EM-wave gravitons.

The entire subject of 'Chemical Kinetics' get altogether a new transparent or absolute shape at this proposition.

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Introduction

The current theories of Chemical Kinetics to a large extent, is unable to provide the true physical concepts regarding the physics and the dimensionalities (or the geometrical shapes) of the rates and rate constants, the order and the activation energies of the chemical reactions.

The principal exercise made in this article is to utilize the definitions of time, mass, volume, EM -wave (electromagnetic wave) etc. of the recently discovered QG theory¹ and to analyse in the light of the said new definitions of the variable (or the said gravitons), the physical parameters of the subject of Chemical Kinetics.

All the Chemical Kinetics' physical parameters get a different newer shape when they are being viewed in regard to 'time Graviton', 'mass graviton', 'volume graviton' and 'EM wave graviton' of the said QG theory.

A QG theory concept driven new definition of Activation Energies of the chemical reactions has been given. This new definition of activation energy has led to develop a new mathematical equation which correlates the following 3 parameters:

- i) Order
- ii) Rate constant
- iii) Activation Energy or Activation volume

As of now no such correlation equation has been reported in the literature and also neither in any of the text books of Physical Chemistry or the literature explain the actual significance of 'order of reaction' or why is it at all being called, 'ORDER'?

The geometrical profile of the chemical reactions of zero, 1st, 2nd, 3rd, etc. have been presented in the pictorial forms.

This work is in fact an unification or blending of the logic and the philosophy of the traditional and the quantum gravity theory.

1.1 Rates of Chemical Reactions, their dimensionalities and Physical Description.

The rate of a chemical reaction is the rate of disappearance of baryonic matters^{2,3} as a function of time. Conventionally it is being expressed as (dc/dt) , where c is the concentration of baryonic matter and t is the time.

The dimension and geometrical shapes of entropy graviton, temperature graviton, time (pull back) graviton, mass graviton, force graviton, energy graviton and electro-magnetic

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wave graviton (EM wave graviton) and an atom (baryonic matter) are shown in Figure 1 below :






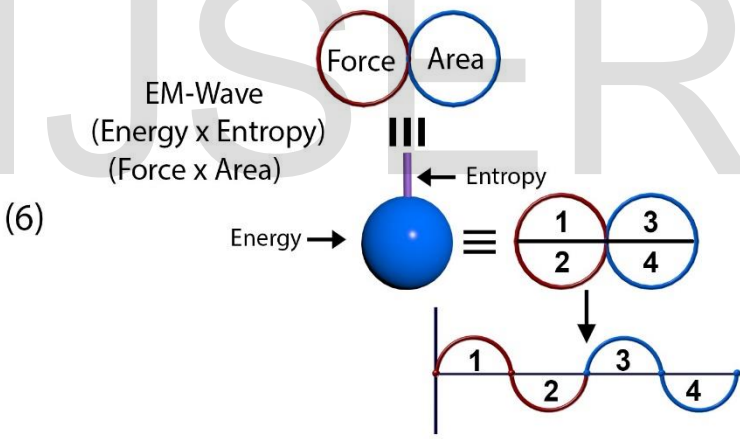
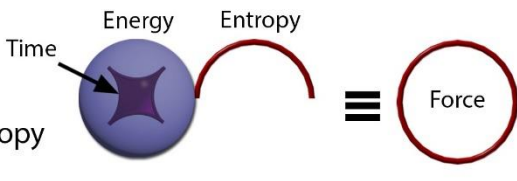
	Graviton Type	Geometrical Shape	Dimension
(1)	Entropy/ Distance	<u>Distance</u>  half circle	$1(r^1)$
(2)	Temperature/Force	 Circle	$2(r^2)$
(3)	Time	 2D Saddle	Inverse $2(r^2)$
(4)	Volume/Energy	 ≡ Sphere	$3(r^3)$
(5)	Mass	 3D Saddle	Inverse $3(r^3)$
(6)	EM-Wave (Energy x Entropy) (Force x Area)		$4(r^4)$
(7)	Atom (Energy x Entropy x Time)	 ≡ Force	$2(r^2)$

Figure 1 : Geometrical Shapes and Dimensions of Gravitons: Entropy, Temperature/Force, Time, Volume, Mass, EM wave and an Atom

From figure 1 it is to follow that while energy/volume (3 dimension) is a hybrid of force and distance, the EM-waves are the hybrids of energy and entropy (4 dimension) and can be represented geometrically as a zone of two nos. of circles or a line emerged out from a 3D sphere or can even be split into the form of typical EM-wave fronts, we are usually accustomed to.

As per QG theory¹, the rate of a chemical reaction, R could be written as:

$$R = r^2 (\text{concentration of baryonic matter}) / (1/r^2) = r^2 \times r^2 = r^4 \quad (1.1)$$

The dimension of the ‘rate’ of a chemical reaction turns out to be 4- dimensional and which resembles the dimensionality of an EM-wave propagation graviton. So, the rate of a chemical reaction or the progress of a chemical reaction is basically EM wave propagation (Figure 1). Speaking in other words, for a chemical reaction to occur, EM wave fronts or EM waves have to flow, in a chemical reaction vessel or mixer.

A baryonic matter can be represented in either of the two following hybridised forms¹:

- i) Energy (r^3) x Entropy(r) x Time ($1/r^2$) (pull back force)
- ii) Mass ($1/r^3$) x Energy(r^3) x Temperature(r^2) (push forward force)

In QG theory¹, ‘Time’ is a ‘pull back force’ and ‘Temperature’ is a ‘push forward force’. The temperature circle on geometrical inversion as described in detail in QG theory¹ is turned to 2-dimensional saddle and which is time. The functions, ‘Time’ and ‘Temperature’ have been established as functions of the universe which are ‘Multiplicative Inverse’ to each other. For example, when one multiplies a variable P, by the multiplicative inverse of the variable ($1/P$), the result is unity and which has no dimension or is dimensionless.

Dividing the above relations i) or ii) by time (an inverse force or inverse square plane) gives rise to situations, the hybrid form of i) or ii) has to overcome an inverse circular plane. This means, the hybridized forms get multiplied by a circular plane (the inverse of a circular plane is a 2-dimensional saddle and its inverse form is a circle or a circular plane) to reach to a different dimension and which is the dimension of an electro- magnetic wave.

Relation i) upon dividing by time turn to

$$\begin{aligned} & \text{Energy x Entropy x Time x Temperature} \\ & = \text{Energy x Entropy (Since time = 1/ temperature)} \\ & = (r^3) \times (r) \\ & = r^4 \text{ (EM wave dimension)} \end{aligned}$$

Relation ii) above upon dividing by time turns to

$$\begin{aligned} & \text{Mass x Energy x Temperature x Temperature} \\ & = (1/r^3) \times (r^3) \times (r^2) \times (r^2) \\ & = r^4 \text{ (EM wave dimension)} \end{aligned}$$

So, it is established that the rates of the Chemical reactions are of EM wave propagation type and the more a chemical reaction progresses more and more EM wave fronts are being generated in a reaction vessel.

The concept underlying this EM- wave generation is, that ‘time’ in fact is an attractive cage, an inverse circle or an inverse force as far as the philosophy of the QG theory is concerned (Sections 3.1, 3.2 and 4 respectively in reference1). For the reactants or baryonic matters or atoms (Section 19.2 and Figure 19.2.1 in reference 1) have to overcome the ‘time attractive cage’ first and then take part in chemical reactions. Overcoming the ‘time attractive cage’ means that the dimension of the atoms/baryonic matters have to overcome an inverse circle. If (x) be the dimension of the baryonic matter and (1/x) being the dimension of time, then once the time dimension is overcome by baryonic matter, the dimension would reach to (x)/ (1/x) or x^2 . In regard to entropy/intermolecular distance (r) terms in QG theory, this x is equal to r^2 and hence x^2 would be equating to r^4 and which is the true dimensionality of EM-wave as per QG theory (Section 8.3 in reference 1).

2.1 ‘Rate Constant’ and ‘Order’ of Chemical Reactions and their Significances.

The order and the rate constants of Chemical reactions are being defined in Chemical kinetics as

rate of a Chemical Reaction,

$$R = k C^n \quad (2.1)$$

Now ‘k’ is the ‘rate constant’ and ‘n’ is the ‘order of the reaction’ and C is the ‘concentration of the reactants’.

If the equation (2.1) is being treated in the light of the QG theory, it becomes,

$$R = r^4 = k x (r^{2n}) \quad (2.2)$$

Equation (2.2) is a general form of representation of the rate constants.

Table 1 represents the dimensionalities of the rate constants in regard to equation (2.2).

By putting $n=0, 1, 2, 3, 4$ respectively for the chemical reactions belonging to different orders, the dimensionalities are being obtained of the rate constants (k) derived from equation (2.2).

Table 1: The Dimensions of the Rate Constants of Chemical Reactions of Different Orders

Order Of Chemical Reaction ‘n’	Dimension of Rate Constant(k) as per Equation (2.2)	Geometrical Shapes of the Rate Constant(k) Gravitons
0	r^4	Hybrid of two numbers of circles or circular planes

1	r^2	A single circle or a single circular plane
2	r^0	Co- existence of one number of a circle and one number of a 2-dimensional saddle. The dimension of the circle is being cancelled by the dimension of the saddle or vice versa and as a result the net dimensionality is zero.
3	r^{-2}	An inverse circular plane or a 2-dimensional saddle or a time graviton.
4	r^{-4}	An inverse EM wave (also referred as anti-magnetic field graviton or a second degree time graviton in QG theory) . This is much squeezing type graviton due the coexistence of two numbers of 2-dimensional saddles of inverse curvature or inverse dimensionality.
5	r^{-6}	Coexistence of two numbers of mass gravitons or second-degree masses.

N.B. For fractional n or order values , for example for n=1.2, k comes out to be $r^{1.6}$ and this can be written in the form say $(r^{0.8})^2$ and $r^{0.8} = R_1$ (say), so the expression of k becomes $(R_1)^2 \dots$ like this.

Figure 2 below, represents the geometrical shapes of the rate constant gravitons of for $n=0, 1, 2, 3, 4$ and 5 .

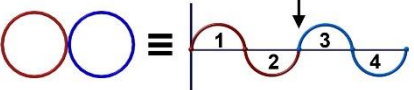





Order of Chemical Reaction (n)	Dimension of Rate Constant(k)	Geometrical Shape of Rate Constant(k)
0	$4(r^4)$	
1	$2(r^2)$	
2	$0(r^0)$	
3	(r^{-2})	
4	(r^{-4})	
5	(r^{-6})	

Figure2 : Geometrical Shape and Dimension of Rate Constant(k) of Zero Order to 5th Order reactions (n=0,1,2,3,4 & 5)

This is being understood very clearly from the data given in Table 1 and the geometrical shapes of the rate constants in Figure 2, that as the order of the reactions become higher , the state of rate constant gravitons become more and more cohesive type or ordered type or squeezing type.

The geometry of the rate constant gravitons, from $n=3$ to $n=5$, for example, as shown in Figure 2, might lead one to believe that the passage available for the reactants (to pass on to the products)in a chemical reaction of order, $n=5$, is the highest among the three. However, the said geometries are being shown in differential forms for better understanding. As a matter of fact , due to the presence of very high level attractive pull back forces in case of $n=5$ (3 nos. 2-dimensional of saddles) compared to the case of $n=3$ (a single 2-dimensional saddle), the integrated form of the rate constant graviton for $n=5$ (3 numbers of saddles will merge to a single saddle of much squeezed size) would be much more lesser than the size of the rate constant graviton in case of $n = 3$. This phenomena has been explained well in the QG theory¹ (Figure A.4.1 in reference 1).

So, through the QG theory only, one can visualize the real physical significance of the lower and higher order of the chemical reactions and the rate constants. Such visualizations were not being possible earlier.

From the above exercise, we do also reach to a very much unified definition of rate constant and order of a chemical reaction and those are given in the foregoing sections.

3.1 Definition of Rate Constant

The rate constant of a chemical reaction is a geometrical passage or space (in the chemical reaction vessel or mixer) and which is the pathway available to the reactants to flow in electro-magnetic wave pattern towards the formation of products.

The shape of the said space or passage is invariant for a certain specific order of reaction. For example, for a zero-order reaction, it has a hybridised shape of two numbers of circles. For a first order reaction it is a circular plane ... and so on like that.

Among several chemical reactions of the same order of reaction (as for example, 3rd order), the size of the said space or passage would be varying but their shapes would remain invariant. If the said shape is as for example be a circle, then the sizes or the areas of the circles would be varying (may be lesser or larger) from one reaction to the other but its shape will remain to be a circle.

For a particular chemical reaction at a constant temperature both the size and shape of the rate constant graviton would remain the same. However, the effect of temperature will be elaborated in the subsequent sections but it is very much obvious to follow that upon increasing the temperature the size of rate constant graviton would be increasing, although the shape will be retained. Since the pathway for the reactants would be wider or larger, upon increasing the temperature, the rate of reactions will increase irrespective of their orders.

4.1 Definition of Order of a Chemical Reaction

The order of a chemical reaction is a specific dimensional graviton that needs to be evolved in a chemical reaction vessel or mixer to transform the dimension of rate constant for that particular order to that of an EM wave graviton form.

For example, in a zero-order reaction, the dimension of rate constant is same to same as that of EM wave dimension. So, no new dimension needs to be created for the zero-order reaction to progress. As a result, zero order reactions do usually progress very fast. Varying the concentration of Baryonic matter has no effect on the rate of chemical reaction since the rate constant graviton is already in the state of a EM -wave dimension.

In a 3rd order reaction, for example, the rate constant graviton is in the form of r^{-2} (a two dimensional saddle). So, to bring it to the level of r^4 , this has to be multiplied by r^6 and which is $(r^2)^3$ or is (concentration of Baryonic matter)³. Hence, we call the order of reaction is 3. The similar logic would be valid for any value of the order, n.

5.1 Significance of Activation Energy of Chemical Reactions in context to the Theory of Quantum Gravity (QG Theory) and its Correlation with Rate Constant and Order of the Chemical Reactions.

The general expression for the rate constant of chemical reaction as per the conventional chemical kinetics is

$$\text{Rate constant} = (\text{litres})^{n-1} (\text{moles})^{1-n} (\text{t}^{-1})$$

Here n is the order of reaction and t is the time in secs.

However, it is to be noted that (1/t) of the above said relation remains to be there irrespective of the order of the reaction is. Since (moles)¹⁻ⁿ is dimensionless, the order of chemical reaction is directly related to (litres)ⁿ⁻¹ or (volume)ⁿ⁻¹.

Table 2: Dimension of Rate Constant (k) as per Conventional Chemical Kinetics

Order of the Chemical Reaction	Dimension of k in regard to (Volume) ⁿ⁻¹ .	Dimension of k in regard to (Volume) ⁿ⁻¹ (t ⁻¹)	Geometrical Shape of Rate Constant (k)
0	(1/ Volume)	(1/ Volume)	The shape cannot be ascertained since the geometry of time has not been defined in Chemical Kinetics
1	(Volume) ⁰	(Volume) ⁰ (sec ⁻¹)	- DO -
2	(Volume) ¹	(Volume) ¹ (sec ⁻¹)	- DO -
3	(Volume) ²	(Volume) ² (sec ⁻¹)	- DO -
4	(Volume) ³	(Volume) ³ (sec ⁻¹)	- DO-
5	(Volume) ⁴	(Volume) ⁴ (sec ⁻¹)	- DO -

The dimension of k as is obtained for the different order of reactions are given in Table 2.

If one does adhere to the dimension as evaluated in the column number 2 of Table 2, it leads to conclude that higher order reactions are more and more random in nature since the dimension of rate constants are increasing from (1/ Volume) to (Volume)⁰ to (Volume)¹ to (Volume)² to (Volume)³ ... so on as one goes from 0 to 1st to 2nd to 3rd ... order reactions respectively. But higher order reactions cannot be more random, it should be more ordered.

So, one is left out with a situation of self- contradictory state of affair and hence such situations could not be explained by the conventional theory of Chemical Kinetics. In contrast to that, one obtains a very good insight of the physics and geometry of the rate constant through QG theory.

Now the parameter 'Activation Energy' of chemical kinetics would be examined. The conventional rate expression of the chemical reactions can now be rewritten as

Rate of chemical reaction = Rate constant x (Baryonic matter concentration)ⁿ

Or, $r^4 = \text{Rate constant} \times r^{2n}$

Or, $r^3 \times r = \text{Rate constant} \times r^{2n}$

Or, Volume = Rate constant x r^{2n-1} (since r^3 represents a dimension of volume) (5.1)

Now the question that arises here that the physical variable 'Volume' in equation (5.1) stands for what? In fact, this is the 'VOLUME FOR ACTIVATION' or 'ACTIVATION ENERGY' for a chemical reaction to take place of order n.

In QG theory 'Volume' (V) is 'Energy' (E) and 'Energy' is 'Volume' and are interconnected to each other as :

$$E = 3V \text{ or } E/V = 3.00 \text{ (under the condition of equilibrium, the pressure, } P = 1)$$

This means that energy density of space is constant. So, equation (5.1) can be rewrite as

Energy of Activation (E_n) of a chemical reaction of order n :

$$E_n = (\text{Rate constant} \times r^{2n-1})/3$$

Or, $E_n = (\text{Rate constant} \times (r^2)^{(n-0.5)})/3$ (5.2)

So, equation (5.2) in a very straight forward manner establishes the relationship between Activation Energy/Activation Volume, Rate Constant, the order and the Concentration of reactants.

If the rate constants for example of a zero order reaction and a 1st order reaction be the same (by magnitude), then for the same concentration of the reactants or baryonic matter the ratio of Activation energies or Activation Volumes (say E_0 and E_1 respectively for zero and 1st order reaction respectively) would be as per equation (5.2) would be

$$E_1 / E_0 > 1 \text{ or } E_1 > E_0$$

So as n goes higher or the order of the reaction be higher, the Activation energy or Activation Volume becomes larger. For zero order reactions the Activation energies are low and as a result the zero-order reaction does progress very fast. An unified definition of Activation Energy or Activation Volume can now be given:

“Activation energy or Activation volume is the optimum volume which needs to be generated in a chemical reaction vessel or mixer for the EM-wave propagation to take place for the formation of the products starting from the reactants or starting from products to reactants “

As shown in Figure 2, the higher the order of chemical reaction, the shapes of the rate constant gravitons become more and more attractive, cohesive or squeezing type. As a result of it, one needs to exert higher and higher push forward forces to generate the said optimum volume as shown below:

Activation Volume or Energy = (Volume compensating to the inverse dimensionality of the Rate Constant + Optimum volume for the EM-wave propagation passage)

If one does have a close look of equation (5.2) and the data provided in Table 1 , the dimensionality of rate constants progressively goes to higher inverse dimensionality (from $n=0$ to 1 to 2 to 3...so on) and which leads to the increase in the value of activation energy (E_n) .

The dimensional analysis and the geometrical profile of zero order, 1st order, 2nd order, 3rd order chemical reactions are given in Figure 3 below


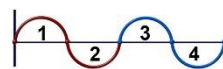


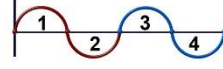


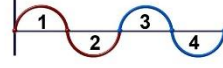


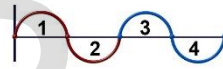
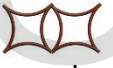

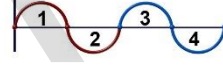


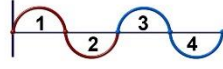
Order of Chemical Reaction (n)	Geometrical Profile of Chemical Reaction		
0		x No Dimension	C^0 
1		x 	C^1 
2	No Dimension 	x 	C^2 
3		x 	C^3 
4		x 	C^4 
5		x 	C^5 

Figure 3 : Geometrical Profile of Zero to 5th Order Reactions ($n=0,1,2,3,4$ & 5 to Generate EM-Wave Pattern (2 Dimensional Saddle being Multiplicative inverse of a Circle, Swallows it, and resulting to a Dimensionless situation).

6.1 The Effect of Temperature on the Rate Constants of Chemical Reactions.

As far as the philosophy of QG theory is concerned, to determine the effect of of temperature on rate constant (k) of the chemical reactions , one should evaluate the results of hybridization of the dimension of rate constant with that of the dimension of temperature. Temperature is a push forward force phenomena (in contrast to time , which is an inverse force or pull back phenomena) having the dimension of r^2 .

In Table 3, the results of hybrid of k and temperature (r^2) have been shown for the various order of the chemical reactions.

Table 3 : Results of Hybridization of the Dimensions of Rate Constants (k) with temperature (r^2) for different order value (n) of the Chemical Reactions

Order of Chemical Reaction 'n'	Dimension of Rate Constant (k) and Temperature (r^2)	Results of Hybrid of Rate Constant (k) and Temperature (r^2)	Comment on the results obtained
0	r^4	r^6	The effect of temperature on rate constant is enormous and the dimension reaches from 4 to 6. A much higher passage is being opened up such that the reaction proceeds much faster as the temperature is being increased
1	r^2	r^4	The dimension of k reaches from 2 to 4 and the reaction becomes quite faster.
2	r^0	r^2	The dimension of k reaches from to 2, reaction rate becomes faster
3	r^{-2}	r^0	The dimension of k reaches from inverse 2 to 0 dimension. The magnitude of rate constant increases.
4	r^{-4}	r^{-2}	The dimension of k reaches from inverse 4 to inverse 2 dimensions. The dimension of k becomes less squeezing or more dispersive type and the rate constant increases.
5	r^{-6}	r^{-2}	The dimension of k reaches to inverse 4 dimensions from inverse 6 dimension. Again, it becomes less squeezing type. In view of the increased passage or space the value

			of rate constant becomes higher.
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From the dimensional analysis given in Table 3 , one can conclude that as the temperature increases the rate constant always increases and the effect is most pronounced for zero order reaction and progressively becomes less and lesser pronounced , higher becoming the value of order of the reactions, due to the effect of more squeezing geometry of the rate constant graviton.

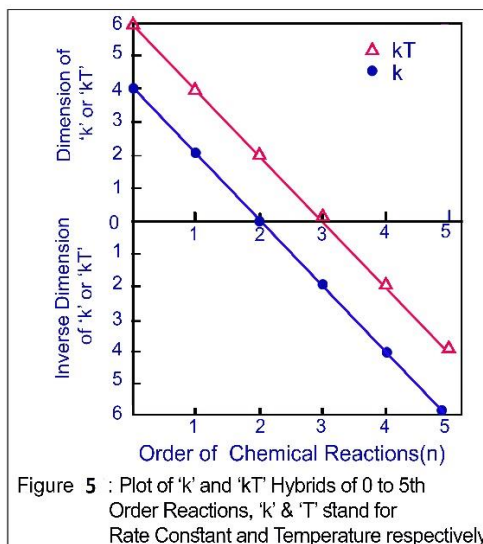
The dimensions and the geometrical shapes of rate constant ‘k’ and ‘k-temperature’ hybrids have been shown side by side for a very distinct comparison between the two. (Figure 4 below):

Order of Chemical Reaction (n)	Dimension of Rate Constant(k)	Dimension of Rate Constant(kT)	Geometrical Shape of (k)	Geometrical Shape of k x r ²
0	4(r ⁴)	6(r ⁶)		
1	2(r ²)	4(r ⁴)		
2	0(r ⁰)	2(r ²)		
3	Inverse 2	0(r ⁰)		
4	Inverse 4 (r ⁻⁴)	Inverse 2 (r ⁻²)		
5	Inverse 6 (r ⁻⁶)	Inverse 4 (r ⁻⁴)		

Figure 4 : Dimensions and Geometrical Shapes of Rate Constant(k) and (kT) Shown side by side

The space in the chemical reaction vessel or mixers for the progress of chemical reaction (in the form of EM-wave graviton) becomes more dispersive or less squeezing type and as a result , the rate constant increases with increase in temperature but the k-temperature coefficient becomes less and lesser positive as n increases.

In Figure 5 below, the dimension of k and k-temperature hybrids have been plotted together against the dimensionality of the Chemical reactions.



From the nature of the plots, the phenomenon of increased dimensionality of k-temperature hybrid is clearly established.

7.CONCLUSION:

The QG theory brings forward, a very clear dimensional picture of the physical parameters of the subject of chemical kinetics like rates and rate constants, the order of the chemical reactions and the activation energies.

These new concepts will help understanding the chemical reaction physics much well and would open up more and more research activities in this and allied fields like chemical thermodynamics, chemical equilibrium and electro-chemistry.

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