ISSN: 0976-5301
Peer Reviewed & Refereed Journal (IF: 7.85)
Journal Website www.coherencejournal.in

EQUATION USING AI TOOLS

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ABSTRACT:

Partial differential equations are widely used in all branches of science. Using PDE to construct mathematical model is a heuristic tool in many areas of sciences. Here in this paper, creation of a new mathematical model using PDE for a discrete data is used to represent a relationship between the various parameters of chemical compounds. We set a formula that connects topological indexes with the Physical properties of chemical compounds, using the above technique.

Keywords: PDE formation, Discrete Data, Scilab programing, Topological index, Mathematical Modelling, AMS classification

INTRODUCTION: Partial differential equations are used in many areas of sciences, like in physics to model heat transfer, wave motion, electricity and magnetism, in Engineering to model fluid motion, stress and strain in structures, in Weather and climate change etc. In physical phenomena, the term "mathematical model" or to be known as a "model/formula" is going to refer to a set of consistent equations intended to explain the particular features or behaviour of a naturally physical system that it seeks to understand [Ado G, Bueno O]. Constructing the partial differential equation as a model, using discrete data is a recent idea. Here in this paper, same procedure of creating a PDE from discrete data is utilised. Further by solving the differential equation a mathematical model or formula representing the data is obtained. A formula that connects topological index with physical properties like melting point, boiling point, viscosity of Alkanes is obtained in this study. Before executing the focused work, a simple problem is solved for verification of the same technique.

As an example, let us consider the function $u(x,t) = \frac{2x}{1+2t}$ in the interval 0<x<1 and t>0. The difference table for u is as follows.

Table 1: gives U(x,t) values in the range x=[0, 1] and t=[0, 5] with equal spacing.

U(x, t)at	T=0	T=0.25	T=0.5	T=0.75	T=1.0
X=0	0.00	0.00	0.00	0.00	0.00
X=0.25	0.50	0.333333	0.25	0.20	0.166667
X=0.5	1.0	0.666667	0.50	0.40	0.3333
X=0.75	1.500000	1.0	0.75	0.60	0.5
X=1.0	2.0	1.333333	1.0	0.80	0.667

Here the data of u(x, t) starting from $x_0=0$ and $t_0=0$, are equally-spaced with h=0.25 and k=0.25, where $x_{i+1}=x_i+h$ and $y_{i+1}=y_i+h$ for i=0,1,2,3,4 . So easily $\frac{\partial u}{\partial x}$ *and* $\frac{\partial u}{\partial t}$ can be obtained. These values are presented in the following table.

Table 2: $\frac{\partial u}{\partial t}$ in each cell.(column wise)

0.000000	0.000000	0.000000	0.000000
-0.666667	-0.333333	-0.200000	-0.133333
-1.333333	-0.666667	-0.400000	-0.266667

-2.000000	-1.000000	-0.600000	-0.400000
-2.666667	-1.333333	-0.800000	-0.533333

Table 3: $\frac{\partial u}{\partial x}$ in each cell.(row wise) the derivative w rt x are

2.000000	1.333333	1.000000	0.800000	0.666667
2.000000	1.333333	1.000000	0.800000	0.666667
2.000000	1.333333	1.000000	0.800000	0.666667
2.000000	1.333333	1.000000	0.800000	0.666667

From above three tables (taking each one as the matrix) will constitute the linear equations, with a b and c as coefficients in the set of linear equations, in the form

$$a\frac{\partial u}{\partial x}(x_1, t_1) + b\frac{\partial u}{\partial t}(x_1, t_1) + cu(x_1, t_1) = 0$$.

….(1)

Then solve these set of linear Partial Differential Equations are solved for the constants a, b, c. For the above data in table1 the partial equations so obtained are,

a*2.000000+b*-0.666667+c*0.333333 =0
a*1.000000+b*-2.000000+c*0.200000 =0
a*2.000000+b*-0.333333+c*0.666667 =0
a*1.000000+b*-1.000000+c*0.400000 =0
a*2.000000+b*-0.200000+c*1.000000 =0
a*1.000000+b*-0.600000+c*0.600000 =0
a*1.333333+b*-1.333333+c*0.250000 =0
a*0.800000+b*-2.666667+c*0.166667 =0
a*1.333333+b*-0.666667+c*0.500000 =0
a*0.800000+b*-1.333333+c*0.333333 =0
a*1.333333+b*-0.400000+c*0.750000 =0
a*0.800000+b*-0.800000+c*0.500000 =0

….(2)

These equations constitute homogeneous equations, out of these equations we choose only the best consistent equations and solve for a, b, c by reducing the matrix of coefficients to the echelon form. By solving the above set of equations we get, the homogeneous system can be written as three representative equations:

$$2a - 0.666667b + 0.333333c = 0,\ a - 2b + 0.2c = 0, 2a - 0.2b + c = 0 \qquad \ldots(3)$$

Hence solving equation (3), we get (a, b, c)=(-8b, b, 50b) Taking (b=1) for a nontrivial solution: **a=-8, b=1, c=50**. With these values all the equations in (2) are approximately satisfied. Hence the PDE by using (1) becomes $u_t - 8u_x + 50u = 0$. Solving this we get

Log(u)=−50t+C and x+8t=C_1 , combining these equations we get

u(x, t) =exp(–50t)f(x+8t) ….(4)

When we compare the values obtained by equation (4), inserting particular function in place of **f** satisfying initial conditions, the values from equation (4) match with the values obtained from original function $u(x,t) = \frac{2x}{1+2t}$, for the same values of x and t. So the same technique is used to find the relations between topological indexes and the physical properties of the alkanes by using ChatGPT tools. For the following table of indexes and physical properties of Alkanes, we apply the above techniques.

Sl no	Formula	Alkane	MV1 – index	VL – index	Melting Point (°C)	Boiling Point (°C)
1	CH_4	Methane	28.3	18	-188	-164
2	C_2H_6	Ethane	49.07	39	-186	-89
3	C_3H_8	Propane	64.54	60	-183	-42

4	C_4H_{10}	*n*-Butane	80.20	81	-38	-1
5	C_5H_{12}	*n*-Pentane	95.94	102	-130	36.1
6	C_6H_{14}	*n*-Hexane	111.75	123	-95	68.7
7	C_7H_{16}	*n*-Heptane	127.59	144	-91	98.4
8	C_8H_{18}	*n*-Octane	143.44	165	-57	125.7
9	C_9H_{20}	*n*-Nonane	159.32	186	-54	150.8
10	$C_{10}H_{22}$	*n*-Decane	175.20	207	-30	174
11	$C_{11}H_{24}$	*n*-Undecane	191.10	228	-10.36	156.58

Lemma 1:The partial differential equation derived, considering u as boiling point and the dependent variable and x-MV1 index, y- VL index, z- Melting point as independent variables is $\mathbf{u_x+1.27u_y+1.08u_z-0.02u=0}$.

Proof: Assume a homogeneous transport-type PDE :$au_x+bu_y+cu_z+du=0$, where u- boiling point, x-MV1 index, y- VL index, z- Melting point Taking a small damping coefficient d=−0.02, we obtain: the derived first-order PDE structure is:
$\mathbf{u_x+1.27u_y+1.08u_z-0.02u=0}$

1. u_x: sensitivity of output to Column 2, MVI index
2. u_y: sensitivity to Column 3, VL index
3. u_z: sensitivity to Column 4, Melting point
4. negative u-term introduces weak decay/stabilization. U- Boiling point

Solving the PDE, we get
u(x,y,z)= exp{0.02x}.F(y-1.27x,; z-1.08x)
Applying First-Row Condition as the initial condition on u(x,yz)= (28.3,18,-188,-164), we get the solved exponential transport solution is:

u(x,y,z)=-93.13e^{0.02x}.(y-0.91x+z)

Where u- boiling point, x-MV1 index, y- VL index, z- Melting point
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