

# Numerical Simulation of the Differential Effect of the Rate of Formation of Vapour Molecules on the Density of Vapour Phase

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**Abstract** – This work considered the effect of the rate of formation of vapour molecules on the density of the vapour phase. The method of analysis is indexed by the numerical method of ordinary differential equations of order 45 (MATLAB ODE 45). It was observed that an increase in the rate of formation of vapour phases resulted in a corresponding increase in the density of vapour molecules. Other novel results which we have not seen elsewhere are presented and discussed quantitatively in this study.

**Keywords** – Vapour Density, Mathematical Quantification, ODE 45, Perturbation.

## I. INTRODUCTION

The scientific construction of developing environmental variables which are inherently uncontrollable and the mathematical models that have been developed by [1] - [8], [10] to understand their evolutions and dynamics do not offer a quick fix intuitive insight. For example, the evolution of the density of vapour phase which depends on sixteen (16) deterministic parameter values according to Sundar [1] is a challenging research problem. To the best of our knowledge, this is an open research problem that requires the application of a mathematical quantification which is called the ordinary differential equation of order 45 (ODE45 numerical simulation).

In an article published by [9], a nonlinear dynamical model was developed. Their model considered the removal of gaseous and particulate pollutants in a rain system using the stability theory of nonlinear ordinary differential equations. One of their key results has shown that under certain conditions, the pollutants can be removed from the atmosphere and their removal rates are subject to the rate of emission of pollutants and other factors. Other research groups in [11] – [15] have considered other parts of related knowledge.

## II. MODEL EQUATIONS

Following Sundar et al (2009), we have considered the following continuous dynamical system of non-linear differential equations of first order:

$$\frac{dC_v}{dt} = Q_v - \mu_0 C_v + \mu_1 \lambda_1 C_d C + \mu_2 C_r C, \quad (1)$$

$$\frac{dC_d}{dt} = \lambda C_v - \lambda_0 C_d - \lambda_1 C_d C, \quad (2)$$

$$\frac{dC_r}{dt} = r C_d - r_0 C_r - r_1 C_r C, \quad (3)$$

$$\frac{dC}{dt} = Q - \delta C - \alpha C C_r + \theta k C_a + \pi v C_a C_r, \quad (4)$$

$$\frac{dC_a}{dt} = \alpha C C_r - k C_a - v C_a C_r. \quad (5)$$

Here, the initial boundary conditions are defined as  $C_v(0) \geq 0$ ,  $C_d(0) \geq 0$ ,  $C_r(0) \geq 0$ ,  $C(0) \geq 0$  and  $C_a(0) \geq 0$  where:

$C_v(t)$  is the density of the vapour phase at time  $t$  in unit of months,

$Q_v(t)$  is the rate of formation of vapour phase in the atmosphere,

$C_d(t)$  is the density of cloud droplets,

$C_r(t)$  is the density of raindrops in the atmosphere,

$C_a(t)$  is the cumulative concentration of gaseous pollutants in the absorbed phase,

$C(t)$  is the cumulative concentration of hot gases in the atmosphere,

$Q$  is the cumulative emission rate of gaseous pollutants,

$\mu_0$  is the natural depletion rate coefficient of vapour phase,

$\mu_1$  is the interaction rate coefficient of cloud droplets and hot gases,

$\mu_2$  is the interaction rate coefficient of raindrops and hot gases,

$r$  is the growth rate coefficient of raindrops due to cloud droplets,

$r_0$  is the natural depletion rate of raindrops,

$r_1$  is the depletion rate coefficient of raindrops due to interaction with hot gases,

$\lambda$  is the growth of cloud droplets formed from the vapour phase,

$\lambda_0$  is the natural depletion rate of density of cloud droplets,

$\lambda_1$  is the depletion rate coefficient of cloud droplets due to interaction with hot gases,  $b$

$\delta$  is the natural removal rate coefficient of hot gases in the atmosphere,

$k$  is the natural removal rate coefficient of gaseous pollutants in the atmosphere,

$\alpha$  is the removal rate coefficient of hot gases due to interactions with raindrops,

$\nu$  is the removal rate coefficient of gaseous pollutants due to interactions with raindrops,

$\theta$  and  $\pi$  are reversible rate coefficients.

$\theta \leq 0$  and  $\pi \leq 1$ .

The following parameter values provided by Sundar were used in this simulation analysis:  $\mu_0 = 2.8$ ,  $\mu_1 = 0.001$ ,  $\mu_2 = 0.001$ ,  $\lambda = 2.5$ ,  $\lambda_0 = 0.1$ ,  $\lambda_1 = 0.8$ ,  $r = 0.8$ ,  $r_0 = 0.7$ ,  $r_1 = 0.01$ ,  $\delta = 0.35$ ,  $\alpha = 0.65$ ,  $k = 0.40$ ,  $\theta = 0.001$ ,  $\pi = 0.00001$ ,  $\nu = 0.50$ ,  $Q = 1$  and  $Q_v = 15$ .

### III. METHOD OF ANALYSIS

For this present study, the evolution of  $C_v$  depends on sixteen (16) deterministic parameters of which the independent variable  $t$  and five (5) initial conditions form the intrinsic deterministic factors that define the evolution of the density of vapour phase  $C_v$  in the atmosphere. In the context of the present model formulation,

each of these model parameter values is varied at 100%. However, in the scenario of environmental modeling, we know that these model parameter values are not static; they can either be decreased or increased. When each model parameter value is varied, what is the expected effect of this variation on the dependent variable called  $C_v$ ? For the purpose of this study, we have utilized the method of ODE45 simulation to study the distinct effects of varying the model parameter value  $Q_v = 15$  on the density of vapour phase  $C_v$ . The new  $C_v$  that is obtained is denoted by  $C_v(\text{new})$ . Whereas, the depleted density of vapour phase when all model parameter values are fixed is denoted by  $C_v(\text{old})$ . For the purpose of clarity, the notation EPD represents the estimated percentage that is depleted whereas the notation EPI represents estimated proportion increase.

#### IV. RESULTS

The full results of this study are presented as shown in Tables 1 - 7 as follows:

Table 1. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v = 0.15$ , on the density of the vapour molecules  $C_v(\text{old})$ : experimented time = 25 months, first row data specify the first month.

Empirical Example	$C_v(\text{old})$ Estimated	$C_v(\text{new})$ Estimated	EPD (%)
1	1.00	1.00	0.00
2	7.54	2.43	67.81
3	9.88	0.73	92.61
4	11.44	0.24	97.88
5	12.23	0.12	99.03
6	12.64	0.09	99.33
7	12.86	0.07	99.44
8	12.99	0.06	99.51
9	13.07	0.06	99.57
10	13.12	0.05	99.60
11	13.16	0.09	99.63
12	13.19	0.05	99.65
13	13.21	0.04	99.66
14	13.23	0.04	99.67
15	13.24	0.04	99.67
16	13.25	0.04	99.67
17	13.27	0.04	99.68
18	13.27	0.04	99.68
19	13.28	0.04	99.68
20	13.29	0.04	99.68
21	13.29	0.04	99.69
22	13.30	0.04	99.69
23	13.30	0.04	99.69
24	13.31	0.04	99.69
25	13.31	0.04	99.69

Table 2. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v = 1.5$ , on the density of the vapour molecules  $C_v(\text{old})$ : experimented time = 25 months, first row data specify the first month.

Empirical Example	$C_v(\text{old})$ Estimated	$C_v(\text{new})$ Estimated	EPD (%)
1	1.00	1.00	0.00
2	7.54	2.88	61.77
3	9.88	1.48	85.07
4	11.44	1.09	90.43
5	12.23	0.10	91.83
6	12.64	0.97	92.31

7	12.86	0.96	92.54
8	12.99	0.95	92.69
9	13.07	0.94	92.81
10	13.12	0.93	92.92
11	13.16	0.92	93.01
12	13.19	0.91	93.11
13	13.21	0.90	93.20
14	13.23	0.89	93.30
15	13.24	0.87	93.40
16	13.25	0.86	93.50
17	13.27	0.85	93.60
18	13.27	0.84	93.70
19	13.28	0.82	93.80
20	13.29	0.81	93.90
21	13.29	0.80	94.01
22	13.30	0.78	94.11
23	13.30	0.77	94.22
24	13.31	0.76	94.32
25	13.31	0.74	94.42

Table 3. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v = 14.25$ , on the density of the vapour molecules  $C_v(\text{old})$ : experimented time=25 months, first row data specify the first month.

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPD (%)
1	1.00	1.00	0.00
2	7.54	7.28	3.50
3	9.88	9.39	5.00
4	11.44	10.83	5.27
5	12.23	11.59	5.27
6	12.64	11.98	5.23
7	12.86	12.20	5.19
8	12.99	12.32	5.15
9	13.07	12.40	5.13
10	13.12	12.45	5.11
11	13.16	12.49	5.10
12	13.19	12.52	5.09
13	13.21	12.54	5.08
14	13.23	12.56	5.07
15	13.24	12.57	5.06
16	13.25	12.58	5.06
17	13.27	12.59	5.05
18	13.27	12.60	5.05
19	13.28	12.61	5.05
20	13.29	12.62	5.04
21	13.29	12.62	5.04
22	13.30	12.63	5.04
23	13.30	12.63	5.04
24	13.31	12.64	5.04
25	13.31	12.64	5.03

Table 4. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v=14.70$ , on the density of the vapour molecules  $C_v(\text{old})$ : experimented time=25 months, first row data specify the first month.

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPD (%)
1	1.00	1.00	0.00
2	7.54	7.43	1.40
3	9.88	9.69	2.00
4	11.44	11.20	2.11
5	12.23	11.98	2.11
6	12.64	12.38	2.09
7	12.86	12.60	2.07
8	12.99	12.72	2.06
9	13.07	12.80	2.05
10	13.12	12.85	2.04
11	13.16	12.90	2.04
12	13.19	12.92	2.03
13	13.21	12.94	2.03
14	13.23	12.96	2.03
15	13.24	12.97	2.03
16	13.25	12.99	2.02
17	13.27	13.00	2.02
18	13.27	13.01	2.02
19	13.28	13.01	2.02
20	13.29	13.02	2.02
21	13.29	13.03	2.02
22	13.30	13.03	2.02
23	13.30	13.04	2.01
24	13.31	13.04	2.01
25	13.31	13.04	2.01

Table 5. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v=15.15$ , on the density of the vapour molecules  $C_v(\text{old})$ : experimented time=25 months, first row data specify the first month.

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPI (%)
1	1.00	1.00	0.00
2	7.54	7.59	0.70
3	9.88	9.98	1.00
4	11.44	11.56	1.05
5	12.23	12.36	1.05
6	12.64	12.78	1.05
7	12.86	13.00	1.04
8	12.99	13.13	1.03
9	13.07	13.20	1.03
10	13.12	13.26	1.02
11	13.16	13.30	1.02
12	13.19	13.32	1.02
13	13.21	13.34	1.02
14	13.23	13.36	1.01
15	13.24	13.38	1.01
16	13.25	13.39	1.01
17	13.27	13.40	1.01
18	13.27	13.41	1.01
19	13.28	13.42	1.01
20	13.29	13.42	1.01

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPI (%)
21	13.29	13.43	1.01
22	13.30	13.43	1.01
23	13.30	13.44	1.01
24	13.31	13.44	1.01
25	13.31	13.45	1.01

Table 6. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v = 15.75$ , on the density of the vapour molecules  $C_v$ (old): experimented time = 25 months, first row data specify the first month.

Empirical Example	$C_{v_p}$ (old) Estimated	$C_{v_p}$ (new) Estimated	EPI (%)
1	1.00	1.00	0.00
2	7.54	7.80	3.50
3	9.88	10.38	5.02
4	11.44	12.04	5.28
5	12.23	12.88	5.27
6	12.64	13.31	5.23
7	12.86	13.53	5.19
8	12.99	13.66	5.15
9	13.07	13.74	5.13
10	13.12	13.79	5.11
11	13.16	13.83	5.10
12	13.19	13.86	5.08
13	13.21	13.88	5.08
14	13.23	13.90	5.07
15	13.24	13.91	5.06
16	13.25	13.93	5.06
17	13.27	13.94	5.05
18	13.27	13.94	5.05
19	13.28	13.95	5.05
20	13.29	13.96	5.04
21	13.29	13.96	5.04
22	13.30	13.97	5.04
23	13.30	13.97	5.03
24	13.31	13.98	5.03
25	13.31	13.98	5.03

Table 7. Assessing the differential effect of the rate of formation of vapour phase in the atmosphere,  $Q_v = 16.2$ , on the density of the vapour molecules  $C_v$ (old): experimented time = 25 months, first row data specify the first month.

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPI (%)
1	1.00	1.00	0.00
2	7.54	7.96	5.60
3	9.88	10.68	8.04
4	11.44	12.40	8.45
5	12.23	13.27	8.44
6	12.64	13.70	8.37
7	12.86	13.93	8.30
8	12.99	14.06	8.25
9	13.07	14.14	8.21
10	13.12	14.20	8.18
11	13.16	14.23	8.15
12	13.19	14.26	8.13
13	13.21	14.28	8.12

Empirical Example	$C_v$ (old) Estimated	$C_v$ (new) Estimated	EPI (%)
14	13.23	14.30	8.11
15	13.24	14.32	8.10
16	13.25	14.33	8.09
17	13.27	14.34	8.08
18	13.27	14.35	8.08
19	13.28	14.35	8.07
20	13.29	14.36	8.07
21	13.29	14.37	8.07
22	13.30	14.37	8.06
23	13.30	14.38	8.06
24	13.31	14.38	8.06
25	13.31	14.39	8.05

### V. DISCUSSION OF RESULTS

The effect of varying the rate of formation of vapour phase ( $Q_v$ ) on the density of vapour phase ( $C_v$ ) is shown in Tables 1 - 7. As seen in Tables 1-2, the density of vapour phase experiences severe depletion for  $Q_v = 0.15$  whereas in Tables 3- 4, the depletion is minimal. As seen in Tables 1 - 2, as the rate of formation of vapour phase is decreased, the density of vapour phase of 67.81% for the second month decreases to 61.77% when  $Q_v = 0.15$  and 1.5 respectively. In Tables 3 - 4, we have observed that for the model parameter values of  $Q_v = 14.25$  and  $Q_v = 14.70$ , the density of vapour phase experiences mild depletion. It decreases from 3.5% for the second month of Table 3 to 1.4% in Table 4. Also, in Tables 5 - 7, the density of vapour phase experiences an increase of 0.70% for the second month (Table 5), 3.50% for the second month (Table 6) and 5.60% for the second month of Table 7.

Further, we have seen that for a twenty-five (25) month numerical simulations, the density of vapour phase depleted when the rate of formation of vapour phase,  $Q_v = 0.14$  is 99.69%. This value decreases to 94.47%, 5.03% and 2.01% respectively.

The implication of this analysis as we have observed in this study is that a decrease in the rate of formation of vapour phase will ultimately lead to increased rainfall and this effect reduces the concentration of gaseous pollutants in the atmosphere. Also, an increase in the rate of formation of vapour phase increases the concentration of gaseous pollutants which is not tractable in environmental science.

It is worth mentioning that Sundar et al (2009) who worked on nonlinear modeling of the interactions of hot gases with cloud droplets and raindrops examined in detail the mathematical ideas of equilibrium analysis and local stability analysis with a few numerical simulations of a specific variation of model parameter values. In their work, a stable unique positive steady state solution was obtained. But in this present analysis, we have clearly used the efficient computational method of ODE 45 numerical simulation to show how the decreasing and increasing variations of the rate of formation of vapour phase  $Q_v$  affect the concentration of vapour molecules  $C_v$  in the atmosphere which has not been previously analysed. Therefore this paper has shown a cutting-edge contribution to knowledge in the scenario of modeling the interactions of hot gases with cloud droplets and raindrops.

However, the present simulated data can be subjected to further data precision, p-vector norms error between interacting data and the Minkowski inequality verification of the interacting data in our future investigation.

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