

3d Scalar Derivatives applied To Interpolation

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Abstract

Until now the only notion we have of a derivative of a scalar field in 3D is the partial derivative where the joint of its components forms the respective gradient corresponding to a conservative vector field, however it is possible to try another alternative that allows us to obtain from the derivative of a scalar function of R^3 another scalar function of R^3 and not a vector, and thus explore other applications. In this work we want to show as the first utility of this scalar derivative in R^3 the advantages in terms of calculation power, simplicity and accuracy, through an example of 3D interpolation commonly used in science and engineering, such as thermodynamic tables of several variables where two of them are independent, and we will compare this process and its result with the traditional method of partial derivatives, We also evaluate the accuracy of the new procedure with the old process, weighing a percentage of error through a simulation in which we interpolate a known value in the table and compare it with the results obtained with both methods.

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I. INTRODUCTION:

The purpose that motivates us in this article is to present, to the scientific-technical community for the first time in the calculus methodology using some scalar derivatives at space R^3 , like as we already did, in due time, with Integral 3D Primitives (Adolfo 2014 Integrales de Simetría), now therefore represent the reverse process. We shall illustrate it with simple application of interpolation in a thermodynamic temperature and pressure table to obtain the specific volume at other intermediate pressure and temperatures. We are going to do it both in 2D and 3D in order to compare them. These tables which are essential for engineering have thermodynamic variables obtained experimentally (gases and real fluids), such as the internal energy "u", entropy "s", enthalpy "h" and the specific volume "v", are tabulated in order to be placed certain values of the independent variable temperature and pressure. Yet it is not possible to place all values of temperature and pressure, hence the need to interpolate the thermodynamic variables for the values of temperature and pressure which are not tabulated. The classic procedure 2D derived for several variables (partial derivatives) carries, usually, the execution of several interpolations: one to find the specific volume (or any thermodynamic variable) varying the temperature at the desired it while maintaining the pressure constant in its first value. A second interpolation is required then for varying the same temperatures while maintaining the pressure constant at the second value. At once obtained the value of the variable for the two pressures at the desired temperature, the last one proceeds to a third interpolation to find the thermodynamic variable to desired intermediate pressure. This is because the mechanism for several variables derivatives 2D, only can vary an amount at a time. We wonder whether will there be a methodology to interpolate, with their respective derivative, varying all variables simultaneously, allowing interpolate the value of the thermodynamic variables sought in one operation? The answer is a resounding yes. This is another advantage that we can score in favor of Integral Symmetry by the fact of having a three-dimensional view of the calculation, ie own definition of the calculation in 3D and not a mere three-dimensional reconstruction by a two-dimensional 2D tool. But first we recall what does interpolation mean.

Interpolation 2D

Interpolation is the mathematical algorithm by which we replace a function $y = f(x)$, whose expression in terms of the argument "x" is unknown or complicated, easier or simpler, say the equation of a line $f(x) = y = mx + b$ (in the case of R^2 plane functions or 2D) to reproduce approximately the dependent variable "and" within a certain limited region values of the variables x, y. In Figure 1 (in yellow shade) we illustrate the equation of the line that replaces the function:

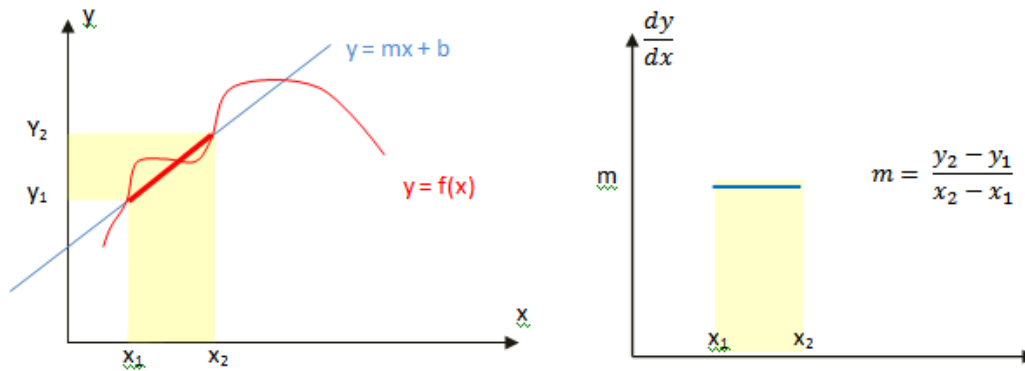


Fig1. In the left shaded area shown in yellow where the function is replaced by a straight lined. In the right the respective value of the slope.

When we interpolate functions of three dimensions of two independent variables $z=f(x,y)$, traditionally apply the same procedure for each variable separately, ie, first to "x", then to "y", then we replace the function $f(x,y)$ by the equation of a plane $z=m_1(x-x_1)+m_2(y-y_2)+z_1$, in Figure 2 illustrate this:

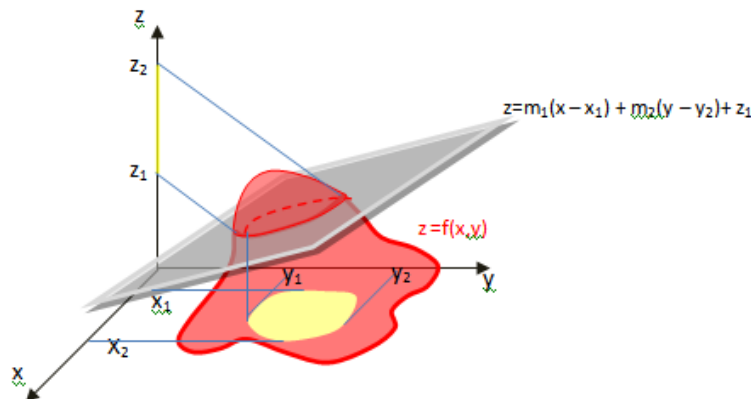


Fig2. Shows the plane which replaces the function in the area where the surfaces intersect.

Our traditional derivative hitherto known, here called 2D, for functions of more than one variable, resulting in a vector designated gradient (∇f) , is not compatible with scalar derivative at three dimensional space we are introducing in this paper. This is because normally address the issues of both two-dimensional and three-dimensional space with a tool that can only process one dimension at a time. While the derivatives synoptic scale 3D allow treatment of the problem, i.e. not limit ourselves to the use of partial derivatives, where one variable varies while other remain constant, but we are talking about a general scalar derivative encompassing the entire process, where all variables are varying simultaneously.

Interpolation 3D

To begin this 3D process the first thing to determine is what kind of expansion we will use among the three expansions that generate 3D primitives, which we have already studied: triangular, round-elliptical and mixed (Adolfo 2014). We evaluated the nature of the function, which can observe qualitatively, that is the volume and its dependence on the two independent variables Temperature and Pressure. It is evident that as the temperature approaches zero (absolute), the volume is reduced (ideally to zero), as well as if the pressure tends to infinity, that is the volume if temperature and pressure at a time. This only means that the variables temperature T and pressure P in the volume function must be expressed as a product, in this case $T \cdot \frac{1}{P}$, by reverse pressure dependence, let's call $\frac{1}{P} = z$. There will be volume when the temperature and the inverse

of the pressure “z” exist simultaneously, $v(T,z) \approx f(T,z)$. TZ. Which means that we are looking for an expansion that generates a product between T and z after integration process, which leads directly to a variable expansion triangular $T, z(p)$ (Adolfo Acosta 2014). Where $f(t, z)$ is an unknown expression of T and z. Figure 3 shows this type of expansion and the appearance of that suggested function:

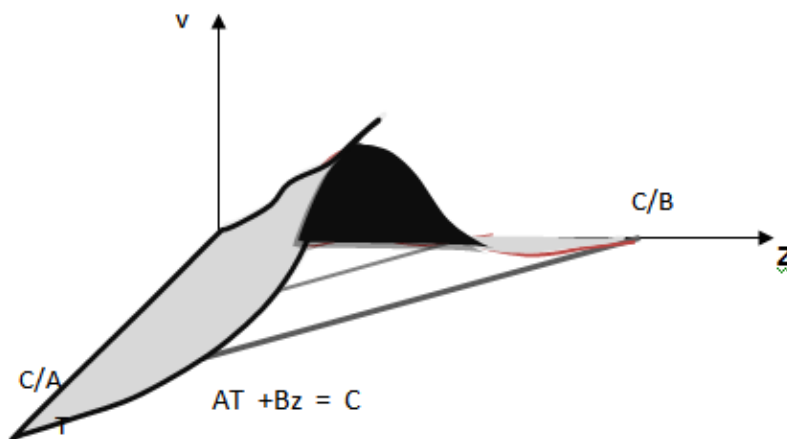


Fig 3. Showing the kind of expansion and surface generated by $v(T,z)$, v is a specific volume function. Where z is the inverse of pressure, $z = 1 / P$

The second thing to determine, once known type variable expansion, is the expansion parameter of these variables. This is necessary because the order of accuracy of the result depends on the variables vary simultaneously under the light of this parameter. As the reader can see in Figure 3 this means that the slope of the line $AT + Bz = C$ is the same straight line ($m = A / B$). I.e. we can take the values of T and $1 / P$ such that $T / (1 / P) = TP \approx \text{constant}$.

Apply this to the next thermodynamic table:

TABLA A.1.3SI (Continuación) Vapor de agua sobrecalentado (unidades SI)												
T	P = 200 kPa (120.23)				P = 300 kPa (133.55)				P = 400 kPa (143.63)			
	v	u	h	s	v	u	h	s	v	u	h	s
900	2.70643	3854.5	4395.8	9.4565	1.80406	3854.2	4395.4	9.2691	1.35288	3853.9	4395.1	9.1361
1000	2.93740	4052.5	4640.0	9.6563	1.95812	4052.3	4639.7	9.4689	1.46847	4052.0	4639.4	9.3360
1100	3.16834	4257.0	4890.7	9.8458	2.11214	4256.8	4890.4	9.6585	1.58404	4256.5	4890.1	9.5255
1200	3.39927	4467.5	5147.3	10.0262	2.26614	4467.2	5147.1	9.8389	1.69958	4467.0	5146.8	9.7059
1300	3.63018	4683.2	5409.3	10.1982	2.42013	4683.0	5409.0	10.0109	1.81511	4682.8	5408.8	9.8780
	P = 500 kPa (151.86)				P = 600 kPa (158.85)				P = 800 kPa (170.43)			
Sat.	0.37489	2561.2	2748.7	6.8212	0.31567	2567.4	2756.8	6.7600	0.24043	2576.8	2769.1	6.6627
200	0.42492	2642.9	2855.4	7.0592	0.35202	2638.9	2850.1	6.9665	0.26080	2630.6	2839.2	6.8158
250	0.47436	2723.5	2960.7	7.2708	0.39383	2720.9	2957.2	7.1816	0.29314	2715.5	2950.0	7.0384
300	0.52256	2802.9	3064.2	7.4598	0.43437	2801.0	3061.6	7.3723	0.32411	2797.1	3056.4	7.2327
350	0.57012	2882.6	3167.6	7.6328	0.47424	2881.1	3165.7	7.5463	0.35439	2878.2	3161.7	7.4088
400	0.61728	2963.2	3271.8	7.7937	0.51372	2962.0	3270.2	7.7078	0.38426	2959.7	3267.1	7.5715
500	0.71093	3128.4	3483.8	8.0872	0.59199	3127.6	3482.7	8.0020	0.44331	3125.9	3480.6	7.8672
600	0.80406	3299.6	3701.7	8.3521	0.66974	3299.1	3700.9	8.2673	0.50184	3297.9	3699.4	8.1332
700	0.89691	3477.5	3926.0	8.5952	0.74720	3477.1	3925.4	8.5107	0.56007	3476.2	3924.3	8.3770
800	0.98959	3662.2	4157.0	8.8211	0.82450	3661.8	4156.5	8.7367	0.61813	3661.1	4155.7	8.6033
900	1.08217	3853.6	4394.7	9.0329	0.90169	3853.3	4394.4	8.9485	0.67610	3852.8	4393.6	8.8153
1000	1.17469	4051.8	4639.1	9.2328	0.97883	4051.5	4638.8	9.1484	0.73401	4051.0	4638.2	9.0153
1100	1.26718	4256.3	4889.9	9.4224	1.05594	4256.1	4889.6	9.3381	0.79188	4255.6	4889.1	9.2049

Table 1. Showing thermodynamic variables v, u, h, s for various values of temperature and water vapor pressure. Courtesy Van Wylen (2012)

Suppose we wish to find the specific volume at a temperature of 180° C and a pressure of 700kpa. As the reader can make sure, these temperature and pressure values are not tabulated, so it is necessary to interpolate. We will do it both 2D and 3D. Recall that the interpolation is to assume that for small variations, the function behaves linearly, i.e. obeys the equation of a line (2D) only in that range of variation, i.e. $v = m_1(T - T_1) + v_1$ where m_1 is the slope ($m_1 = \frac{\partial v}{\partial T} = \frac{v_2 - v_1}{T_2 - T_1}$). Or likewise now varying the pressure $v = m_2(P - P_1) + v_1$ where ($m_2 = \frac{\partial v}{\partial P} = \frac{v_2 - v_1}{P_2 - P_1}$). These lines also contain the plane tangent to the surface of v . Then the linear function that replaces the original function of the specific volume from T_1, Z_1 is:

$$v = m_1(T - T_1) + m_2(z - z_1) + v_1$$

v_1 is volume corresponding at T_1 and $P_1(1/z_1)$. In Figure 4 we illustrate the 2D interpolation of three-dimensional problem.

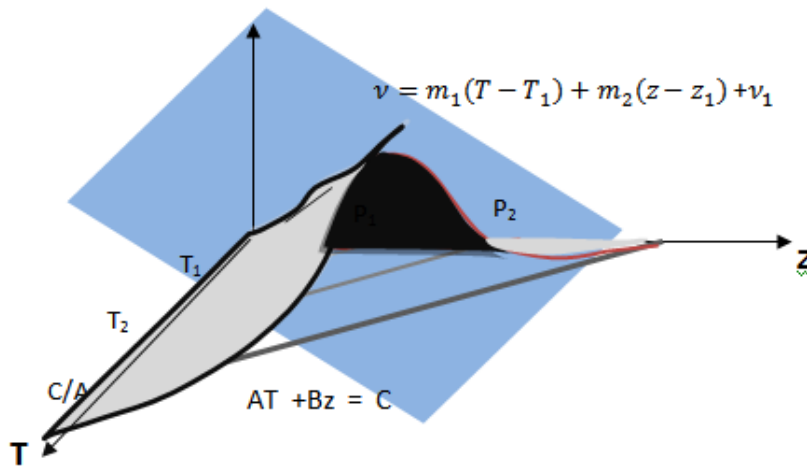


Fig4. Graphically showing the 2D procedure that fits a plane to the surface of $v(T, Z)$

Now in 3D will also make the assumption that the function is linear. Here linear means that the derivative in the triangular expansion is constant, corresponding to the function $z = f(x, y) = xy/2$ (Adolf 2014p.39 and 92) only in the spatial domain represented by a prism containing the values T_1, T_2, P_1 and P_2 as a base and the slope as height, see figure 5. Thus the linear function that replaces the original function from the line through T_1, P_1 (corresponding to the plane $AT + Bz = C_1$) to T_2, P_2 (plane $AT + Bz = C_2$) is:

$$v = m(T.z - T_1 z_1) / 2 + v_1$$

Where $m = \frac{v_2 - v_1}{(T_2 z_2 - T_1 z_1) / 2} \approx \frac{dv}{d_s^{\Delta} T z}$

This according to derivative notation 3D, where Δ means that the derivative is triangular expansion and "s" Integral of Symmetry (Adolfo 2014p.35 and 92) and $Z = 1 / P$ (reverse pressure). Both in Figure 5 illustrate the primitive of the expansion $v = m(T.z - T_1 z_1) + z_1 = g(T, z)$ and the prism representing the respective triangular derivative with the interpolation.

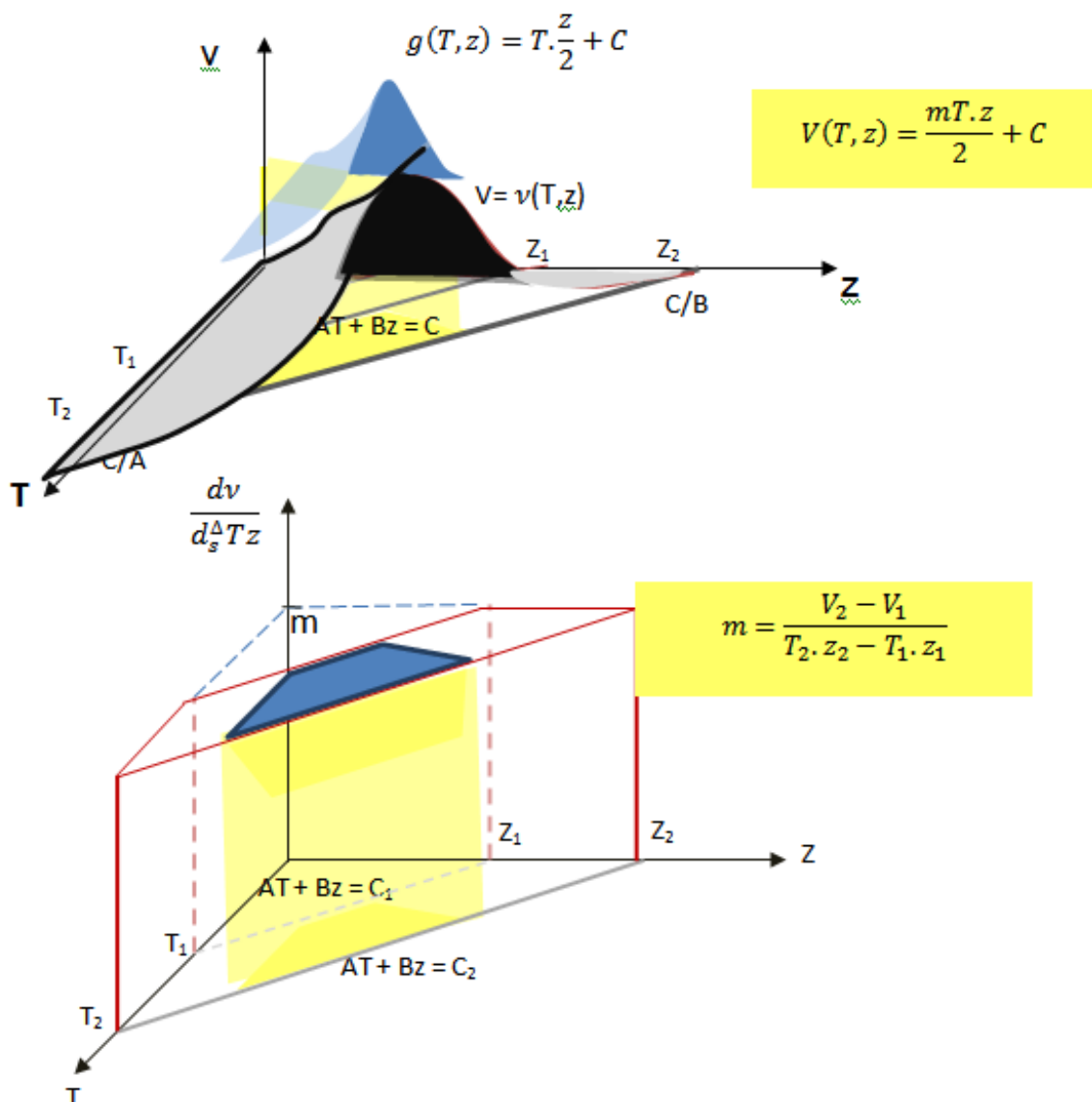


Figure 5. Showing the 3D graphically procedure adjust the surface $G(t, z) = Tz/2$ on the surface of $v(T, Z)$. The prism below corresponds to the triangular derivative with surface $G'(t, z) = m$. They work only in yellow shadow.

Let's show below the respective calculations in 2D and 3D.

2D

1. Holding pressure at 600Kpa

T	v
T ₁ = 158°C	0.31567
T = 180°C	x=?
T ₂ = 200°C	0.35202

$$x = \frac{0.35202 - 0.31567}{200 - 158} (180 - 158) + 0.31567$$

$$x = v_1 (180,600) = 0.32412$$

2. Holding pressure at 800Kpa

T	v
T ₁ = 170°C	0.24043
T = 180°C	x=?
T ₂ = 200°C	0.2608

$$x = \frac{0.2608 - 0.24043}{200 - 170} (180 - 170) + 0.24043$$

$$x = v_2 (180,800) = 0.24496$$

3. Holding Temperature at 180°C

P	v
P ₁ = 600	0.32412
P = 700	x=?
P ₂ = 800	0.24496

$$x = \frac{0.24496 - 0.32412}{800 - 600} (700 - 600) + 0.32412$$

$$x = v (180,700) = 0.28454$$

3D

T	P	v	T.P	Area = T.z
T ₁ = 431K	P ₁ = 600Kpa	0.31567	259110	0.71972
T = 453K	P = 700Kpa	x=?	317100	0.647142
T ₂ = 473K	P ₂ = 800Kpa	0.26080	378400	0.59125

$$x = v = \frac{0.2608 - 0.31567}{0.59125 - 0.71972} (0.647142 - 0.71972) + 0.31567$$

The numbers "2" (Fig 5) have been cancel between them

$$x = v (180,700) = 0.28467$$

Note: We are working in Kelvin degrees (K = 273 + °C)

To check the accuracy of this methodology also let's interpolate with the same procedure, an intermediate value of the specific volume that appears in the table, for instance P=600kPa and T =400°C, corresponding to a value of v=0.51372 as we can see in the table.

	P = 500 kPa (151.86)				P = 600 kPa (158.85)				P = 800 kPa (170.43)			
Sat.	0.37489	2561.2	2748.7	6.8212	0.31567	2567.4	2756.8	6.7600	0.24043	2576.8	2769.1	6.6627
200	0.42492	2642.9	2855.4	7.0592	0.35202	2638.9	2850.1	6.9665	0.26080	2630.6	2839.2	6.8158
250	0.47436	2723.5	2960.7	7.2708	0.39383	2720.9	2957.2	7.1816	0.29314	2715.5	2950.0	7.0384
300	0.52256	2802.9	3064.2	7.4598	0.43437	2801.0	3061.6	7.3723	0.32411	2797.1	3056.4	7.2327
350	0.57012	2882.6	3167.6	7.6328	0.47424	2881.1	3165.7	7.5463	0.35439	2878.2	3161.7	7.4088
400	0.61728	2963.2	3271.8	7.7937	0.51372	2962.0	3270.2	7.7078	0.38426	2959.7	3267.1	7.5715
500	0.71093	3128.4	3483.8	8.0872	0.59199	3127.6	3482.7	8.0020	0.44331	3125.9	3480.6	7.8672
600	0.80406	3299.6	3701.7	8.3521	0.66974	3299.1	3700.9	8.2673	0.50184	3297.9	3699.4	8.1332
700	0.89691	3477.5	3926.0	8.5952	0.74720	3477.1	3925.4	8.5107	0.56007	3476.2	3924.3	8.3770
800	0.98959	3662.2	4157.0	8.8211	0.82450	3661.8	4156.5	8.7367	0.61813	3661.1	4155.7	8.6033
900	1.08217	3853.6	4394.7	9.0329	0.90169	3853.3	4394.4	8.9485	0.67610	3852.8	4393.6	8.8153

It's pretend we do not know this value, let's interpolate both in 2D and 3D:

2D	
1. Holding pressure 500Kpa	
T	v
T ₁ = 300°C	0.52256
T = 400°C	x=?
T ₂ = 600°C	0.80406
$x = \frac{0.80406 - 0.52256}{600 - 300} (400 - 300) + 0.52256$	
$x = v_1(400, 500) = 0.6164$	
2. Holding pressure 800Kpa	
T	v
T ₁ = 300°C	0.32411
T = 400°C	x=?
T ₂ = 600°C	0.50184
$x = \frac{0.50184 - 0.32411}{600 - 300} (400 - 300) + 0.32411$	
$x = v_2(400, 800) = 0.38335$	
3. Holding Temperature 400°C	
P	v
P ₁ = 500	0.6164
P = 600	x=?
P ₂ = 800	0.38335
$x = \frac{0.38335 - 0.6164}{800 - 500} (600 - 500) + 0.6164$	
$x = v(400, 600) = 0.53871$	

3D				
T	P	v	T.P	Area = T.z
T ₁ = 573K	P ₁ = 800Kpa	0.32411	458400	0.71625
T = 673K	P = 600Kpa	x=?	403800	1.1217
T ₂ = 873K	P ₂ = 500Kpa	0.80406	436500	1.746
$x = v = \frac{0.80406 - 0.32411}{1.746 - 0.71625} (1.1217 - 0.71625) + 0.32411$				
The numbers "2" (fig 5) have been cancel between them				
$x = v(400, 600) = 0.513068$				
Note: We are working in Kelvin degrees (K = 273 + °C)				

II. CONCLUSIONS

The advantages of the new procedure in 3D are obvious, first to the accuracy of the result with percentage error of (0.51372 to 0.513068) / 0.51372 · 100% = 0.1% compared to the error of (0.51372 to 0.53871) / 0.51372 · 100% = 5% (50 times) committed with the regular procedure. So we can state categorically that this method of calculation is more attached to the behavior of nature. In essence, this is because the effectiveness resulting from adjusting the surface specific volume $v(t, z)$ shown in Figure 3, with a surface $G(T, z) = Tz + C$, rather than setting it as a plane with the 2D method of partial derivative. Secondly, we also highlight the fact that the 3D entered data procedure are less since only a temperature is necessary for each pressure (one by one). Instead the ordinary procedure requires introducing the two temperatures for each respective variable pressure and the other thermodynamic variable obtained in each case. However we must remember that this procedure has this performance provided the variable temperature and pressure vary simultaneously under the same parameter expansion, or at least about, so when we are far from this requirement will continue using the conventional method. We finally ended up saying that this procedure is just the beginning of what is achieved in the first approximation of a function of several independent variables that can be expressed in a power series in 3D.

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