BACK

Ideal Gas - Real Gas using DERIVE

(Johann Zöchling, Berndorf, Austria)

1. Introduction

Thermodynamics lessons usually bore the pupils aged from 15 to 16. The introduction of experimental equipments for students has been raising their interest in some fields of thermodynamics, e.g. special heat capacity of metals or alloys, thermal conductivity, radiation heat transfer.....
Due to the lack of money, but mainly because of the risk of breaking glass, experiments concerning the dynamics of a gas are restricted to the teacher. Pupils used to doing experiments on their own are normally uninterested in watching experiments done by their teacher. Therefore we tried last year to do some experiments concerning gas dynamics with "computer algebra", especially with DERIVE.
The two most important aims were:

a) *the visualization of the ideal gas equation of state*

b) *to expand the equation of ideal gases to an equation of real gases*

The didactic aims were:

a) to give a deeper insight into what is happening in gases.
b) to train the pupils to model physical equations.
c) to show the efficiency and the limits of physical models.

the organization of work:

Because of the small number of pupils in class (only 14), we had no problems of organization.
Each pupil was working alone with a copy of DERIVE.
Results of calculations and plots were printed and glued down in the exercise books.
The time needed to complete the work was about 2 weeks
(3 lessons a week).

2. The visualization of the ideal gas equation of state

2.1) Theoretical preparatory work

We developed with the help of simple classical mechanics (momentum conservation, Boltzmann's equipartition principle of energy) a pressure - volume - temperature relationship of an ideal gas. We also introduced Avogadro's number and defined the quantity mole.
We used 3 versions of the ideal gas equation of state:

$$a)\ pV = NkT$$
$$b)\ pV = nRT$$
$$c)\ pV_m = RT$$

p....pressure
V....enclosed volume of the gas
T....absolute temperature
k....Boltzmann's constant
R....ideal gas constant
n....number of moles
V_m..volume per mole

The pupils also learned the well known relationships

of *Boyle-Mariotte*	$d)$	$pV = const$
of *Gay-Lussac*	$e)$	$V = const\ T$
and of *Jaques Charles*	$f)$	$p = const\ T.$

They drew the usual plots (isotherms,isobars,isochors) and calculated some problems.

After a few lessons during a short examination one pupil said:

"There are four ideal gas equations of state; a big one (a,b,c), which is more or less useless and 3 small ones (d,e,f). With the small ones we can solve most of our problems. The small ones are also nice and easy to draw"

The connection between (a,b,c) and (d,e,f) was completely lost.
With the help of DERIVE we tried to recover this connection. We tried to draw the "big one" and to find the "small ones" in this plot.

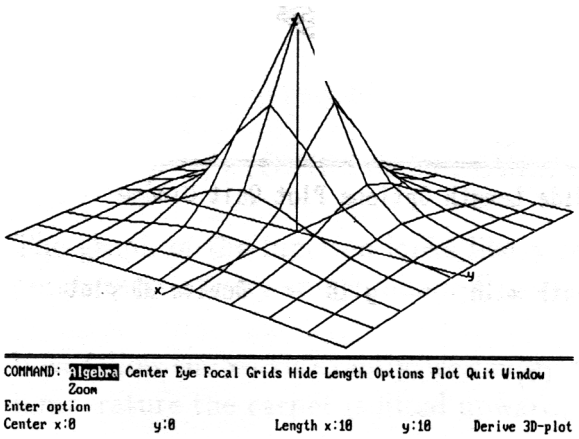
2.2 Working with DERIVE

First we plotted some functions like z = f(x,y) defined in a closed rectangle region of the xy-plane $-a \leq x \leq +a$,
bzw.$-b \leq y \leq +b$. Because of the variation of the grid the pupils knew very well the inaccuracy of the plot.
Example:

$$z = \frac{1}{x^2 + y^2 + 2}$$

$$-5 \leq x \leq 5, -5 \leq y \leq 5$$

DERIVE:
AUTHOR: $z = 1/(x^2 + y^2 + 2)$
PLOT
LENGTH *x:10 y:10 z:10*
GRIDS *x:10,5,50 y:10,5,50*
PLOT



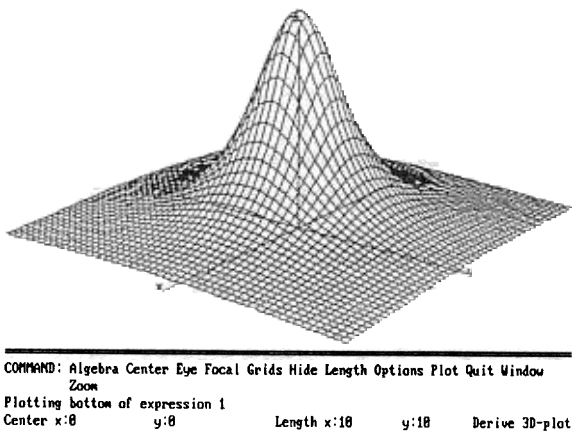


Fig. 2.1: $z = \frac{1}{x^2+y^2+2}$ ($10x10$ grid) Fig. 2.2: $z = \frac{1}{x^2+y^2+2}$ ($50x50$ grid)

The ideal gas equation of state

DERIVE:
AUTHOR: $pv = rt$
DECLARE:*variable: r, value: 1*
SOLVE: *Nr.1, variable p*
PLOT
LENGTH: *10,10,10*
CENTER: *5,5,0*
GRIDS : *20,20 - 50,50*
EYE : *25,20,15*
PLOT

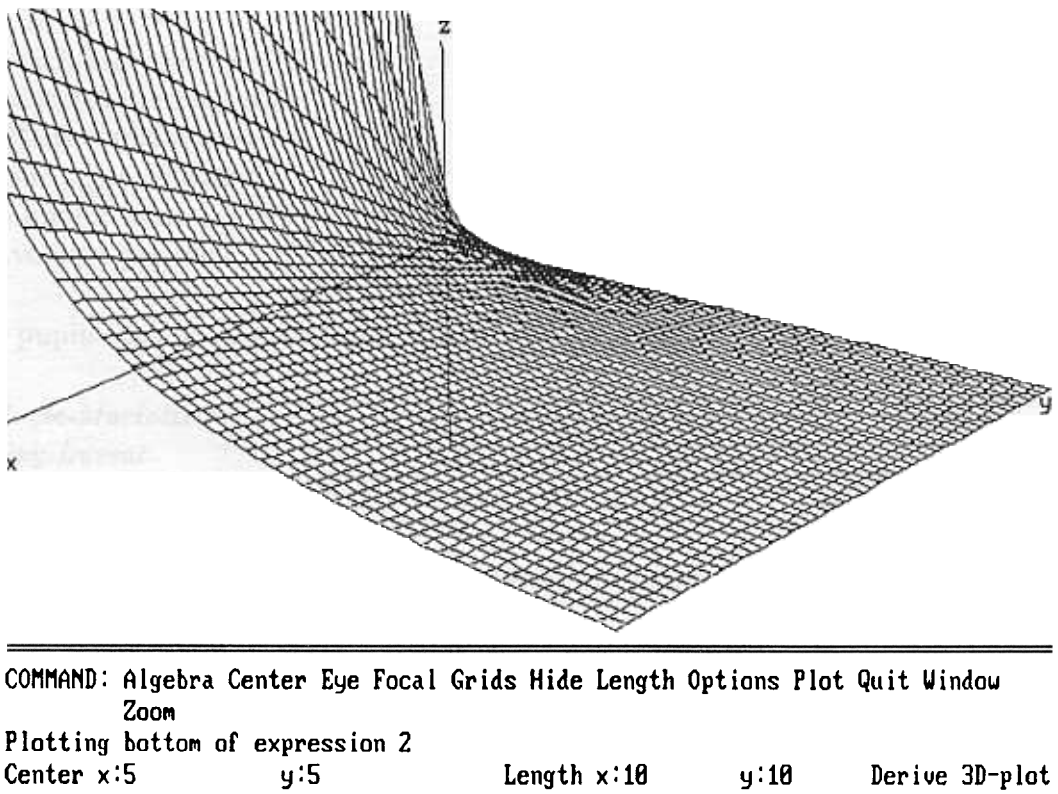


Fig. 2.3: p=t/v (GRIDS:50,50 , EYE:25,25,15)

DERIVE's graphics screen shows a wire frame model of the equation of state. The x-axis is equivalent to the temperature, the y-axis to the volume and the z-axis to the pressure. Each point on this surface shows a definite state of p-V-T of the ideal gas.

Several times we change the point of view now to get a better impression of the shape of the function.

We are following the x-axis:

DERIVE :
EYE: *25,0,5 - 25,5,5*
PLOT

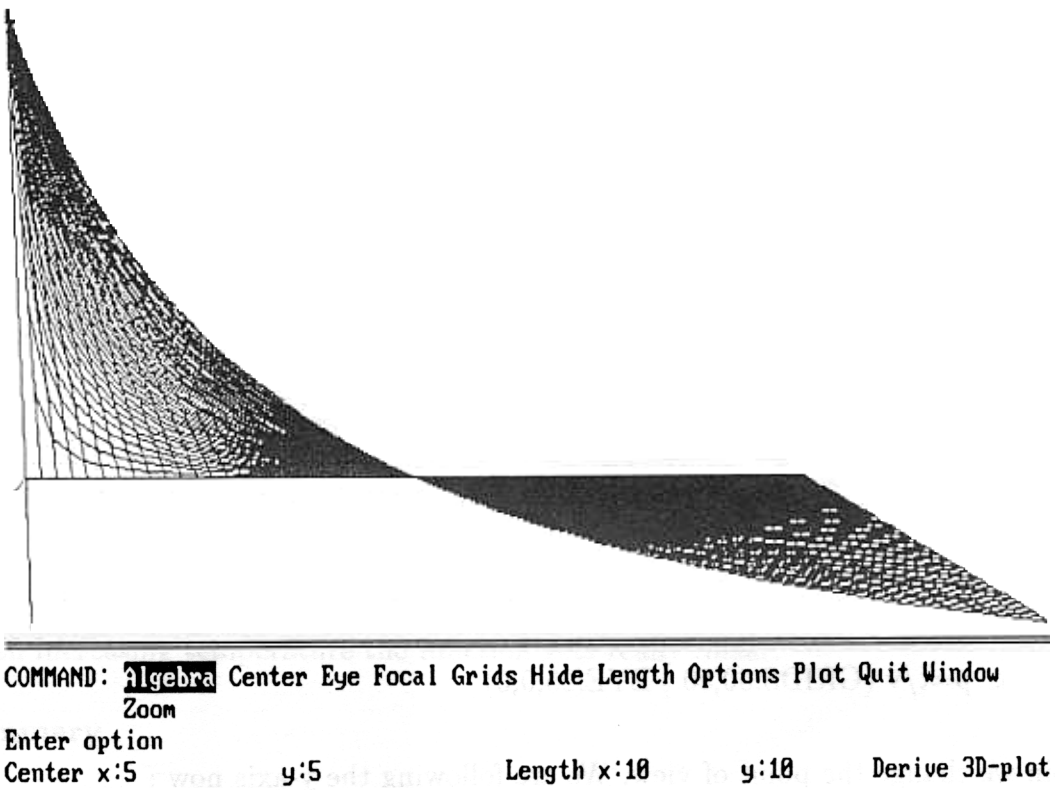


Fig. 2.4 p=t/v (GRIDS:50,50 , EYE:25,5,5)

The graph of the function looks like a carpet which is lifted upward near the temperature axis (very small volume !!), denoting high values of pressure in this region.

If we follow the x-axis exactly, we can see the bottom of the function. With increasing temperature the carpet is lifted upward, probably linearly.

DERIVE:
EYE: *25,0,0*
PLOT

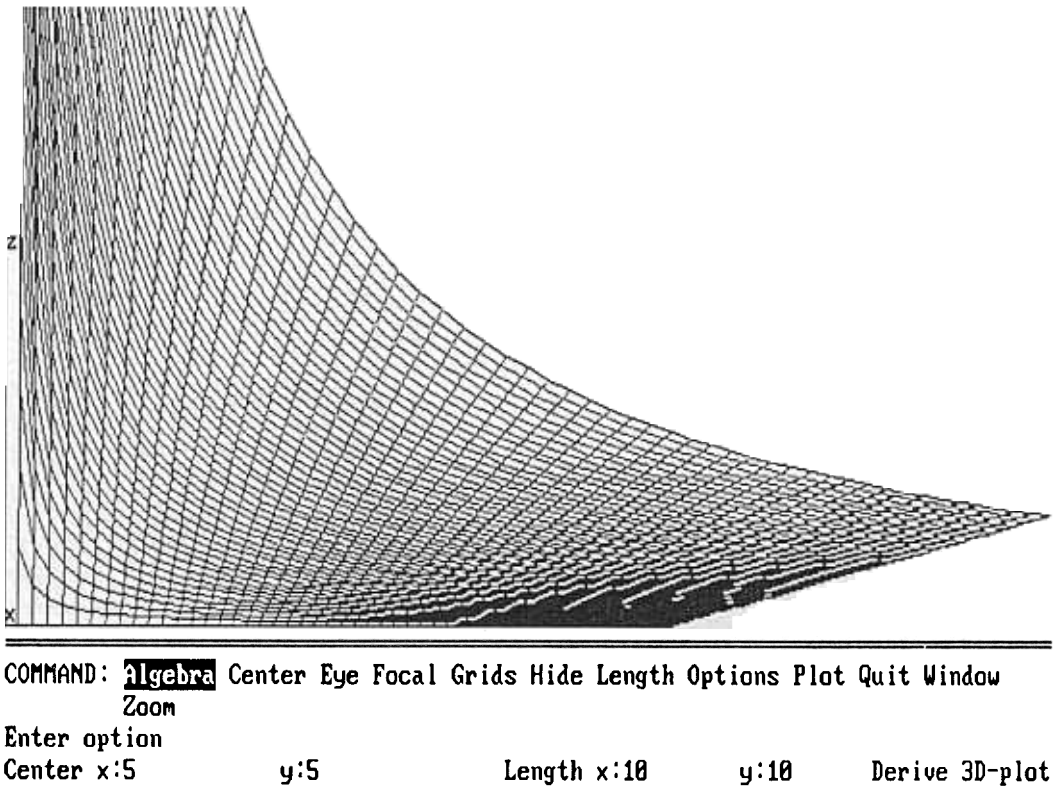


Fig. 2.5: p=t/v (GRIDS:50,50 , EYE:25,0,0)

Again we change the point of view. We are following the y-axis now :

DERIVE:
EYE:*0,25,0*
PLOT

It's also possible to choose other values for "EYE", e.g.(3,25,0)etc.

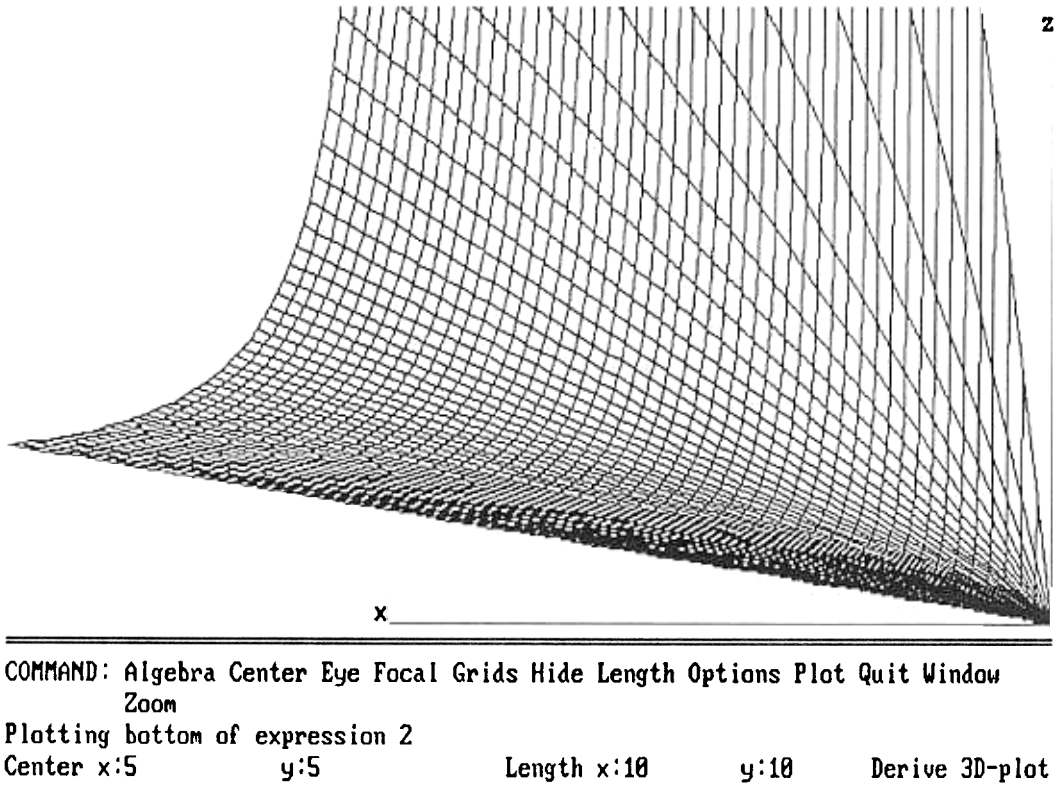


Fig. 2.6: p=t/v (GRIDS:50,50 , EYE:0,25,0)

With increasing temperature the function gets really linear.

summary

What can we learn from the plot of the ideal gas equation of state ?

a) Each relationship between pressure, volume and temperature is characterized by a point on the surface of the function.
b) Moving along a gridline parallel to the temperature axis (constant volume !), pressure is increasing linearly.
This behaviour reminds us of the isochors.
c) Moving along a gridline parallel to the volume axis (constant temperature !), pressure is increasing in a nonlinear way.
This behaviour reminds us of the isotherms.

Where are the isotherms and isochors on the pVT-surface ?

First of all we draw a new pVT-surface based on a rectangular grid.
DERIVE:
GRIDS: 10,20
We project the gridlines of constant temperature on the y-z-plane.
We define a vector: [1/v,2/v,3/v,4/v,5/v,6/v,7/v,8/v,9/v,10/v]
and split the screen into three windows.
window 1: text:"vector"
window 2: 3-D-plot
window 3: 2-D-plot

The plot of window 3 shows the wellknown isotherms.

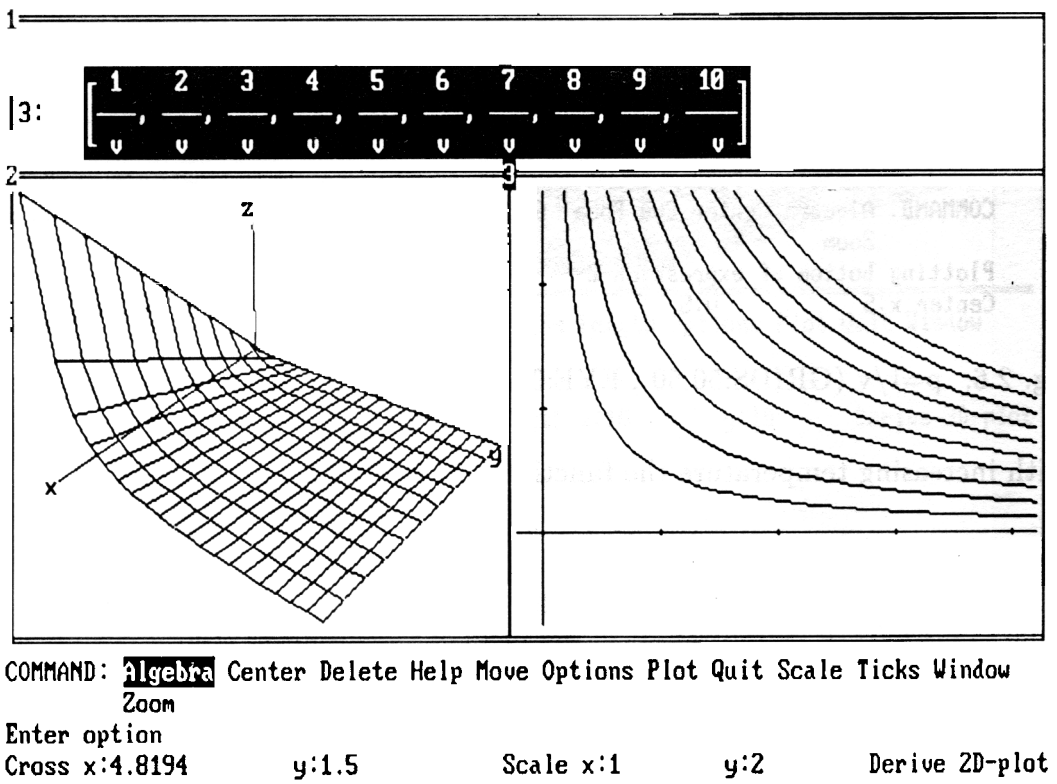


Fig. 2.7: 3-D-Plot:p t/v 2-D-Plot of the isotherms

In the same way we receive the isochors:
We plot a pVT-surface with a grid of (10x5) and project the gridlines parallel to the x-axis on the x-z-plane. We again define a vector [t,t/2,t/3,t/4,t/5] for the projection.

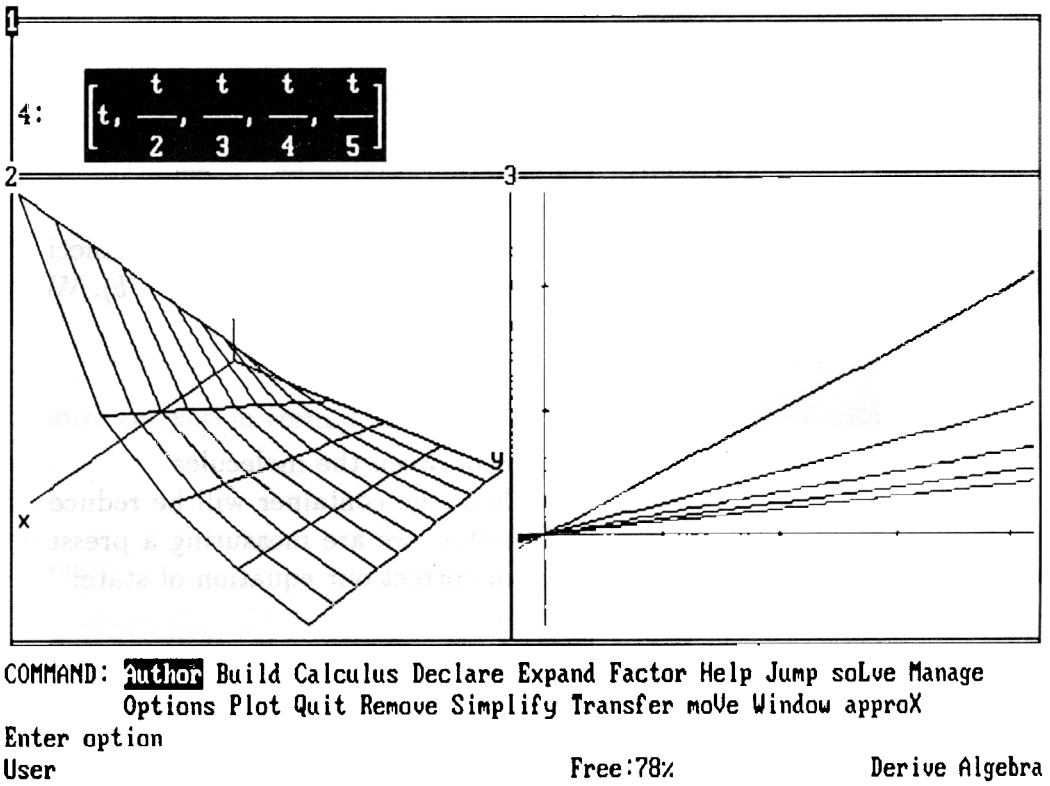


Fig. 2.8: 3-D-plot:$p = t/v$ 2-D-plot of the isochors

3. An "equation" for real gases

3.1 theoretical consideration

As the term suggests, an ideal gas is an idealized model, which represents the behaviour of gases very well in some circumstances, less well in others. We made some simplifications:
a) the volume of the molecules is negligibly small.
b) there are no interactions between the molecules.

We are trying to correct our ideal gas equation, taking into account the volume of the molecules as well as the interactions.
The volume of a molecule is to be v, the sum of the volumes of all molecules is to be b. Therefore the free volume for all particles is reduced to $(V_m - b)$. We correct our equation of state:

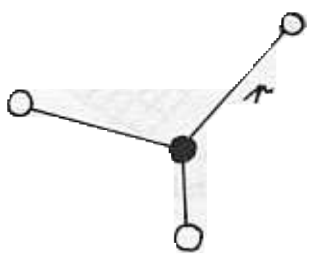
$$p(V_m - b) = RT$$

Next we take into account the interactions between the molecules.
The pressure of a gas exerted on the walls of the container will be reduced due to the attractive force of the molecules. Therefore we are measuring a pressure lower than the real pressure in the gas. We again correct our equation of state:

$$(p + p')(V_m - b) = RT$$

What can be said about p' ?

The potential energy of the interaction between two molecules is to be $E(r)$.



The total potential energy exerted on one molecule is :

$$E_{sum} = \sum_{i=1}^{N-1} E(r_i)$$

We don't know any value of E_{sum}. All we know is a direct proportion between E_{sum} and the number density of the gas $\frac{N}{V}$.

$$E_{sum} = \frac{N}{V} K \quad (K...constant)$$

Taking into account the interactions between all molecules and counting interactions between two molecules only once
(factor $\frac{1}{2}$), we receive for the sum of the energy:

$$E_{sum} = \frac{1}{2} \frac{N(N-1)}{V} K \approx \frac{N^2}{V} K'$$

Therefore the attractive forces of the molecules change the energy of the gas. Changing the energy results in a change of pressure.

$$p = \frac{E}{V}$$

the pressure correction term p' is then:

$$p' = \frac{N^2}{V^2} K'$$

using moles:

$$n\, N_A = N$$

n....number of moles
N_A..Avogadro's/Loschmidt's-constant

we can write:

$$p' = \frac{a}{{V_m}^2}$$

Our new, refined equation of state is then:

$$(p + \frac{a}{{V_m}^2})(V_m - b) = RT$$

What can we do with this equation ?

(comment: Using DERIVE we write V instead of V_m)

Let's now investigate the behaviour of the new equation.
We restrict ourselves to the 2-D-plots of the isotherms.

3.2 Working with DERIVE

As we are only interested in the qualitative behaviour of our equation, we choose arbitrary values for the constants a and b.
a=1, b=0.1

DERIVE
AUTHOR:$(p + a/v^2)(v - b) = rt$
DECLARE: *variable: a, value 1*
DECLARE: *variable: b, value 0.1*
DECLARE: *variable: r, value 1*
SOLVE: *Nr.1, variable p*
EXPAND: *"all"*

now we choose different values for t and plot the isotherms:
DERIVE
DECLARE: *variable: t, value 10,15,5,2.5*
PLOT

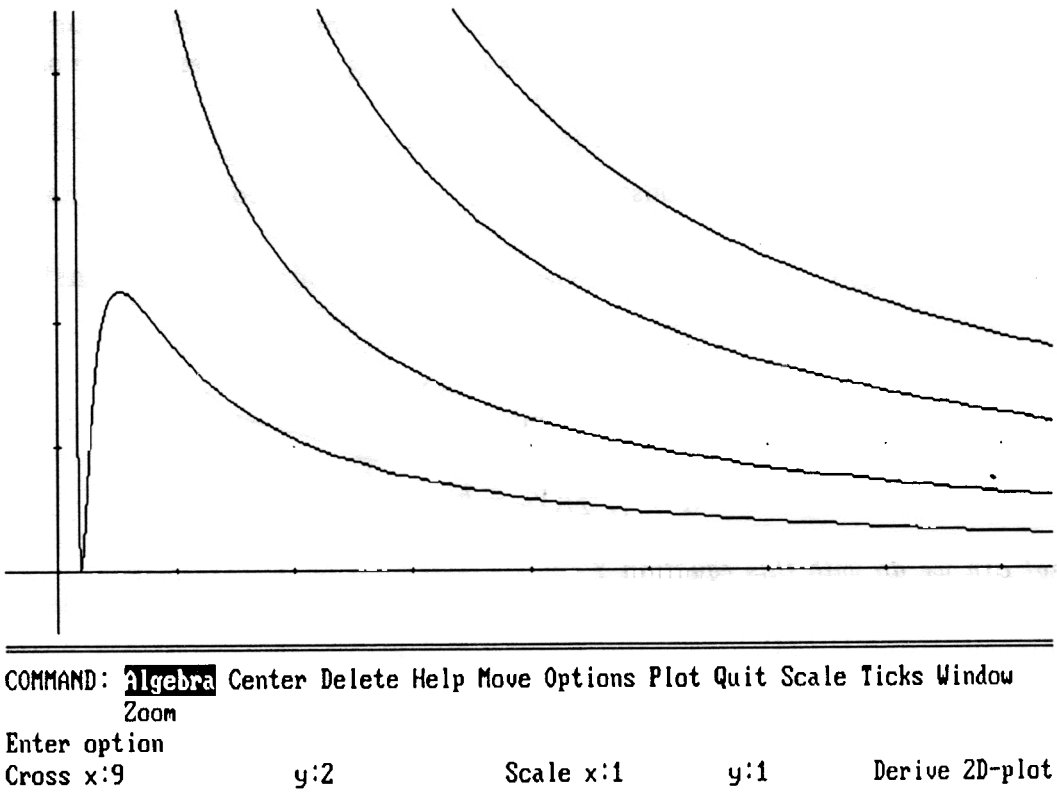


Fig.3.1: isotherms for t=10,15,5,2.5

For t=10, 15 respectively 5 we receive isotherms, similar to those of the ideal gas. The isotherm of t=2.5 is completely different from the well known isotherms of the ideal gas.
Using a vector we plot now the isotherms in the "critical region " between t=2.5 und t=5.
With the help of the ZOOM option we magnify the critical region. (Fig.3.2,3.3)

DERIVE
DECLARE: *function: pr , value:* $\frac{10t}{10v-1} - \frac{1}{v^2}$
AUTHOR: *[pr(2.5,v),pr(.....]*
PLOT

We plot again the isotherms using different scaling for the y-axis.
(e.g. SCALE y:5).(Fig.3.4)

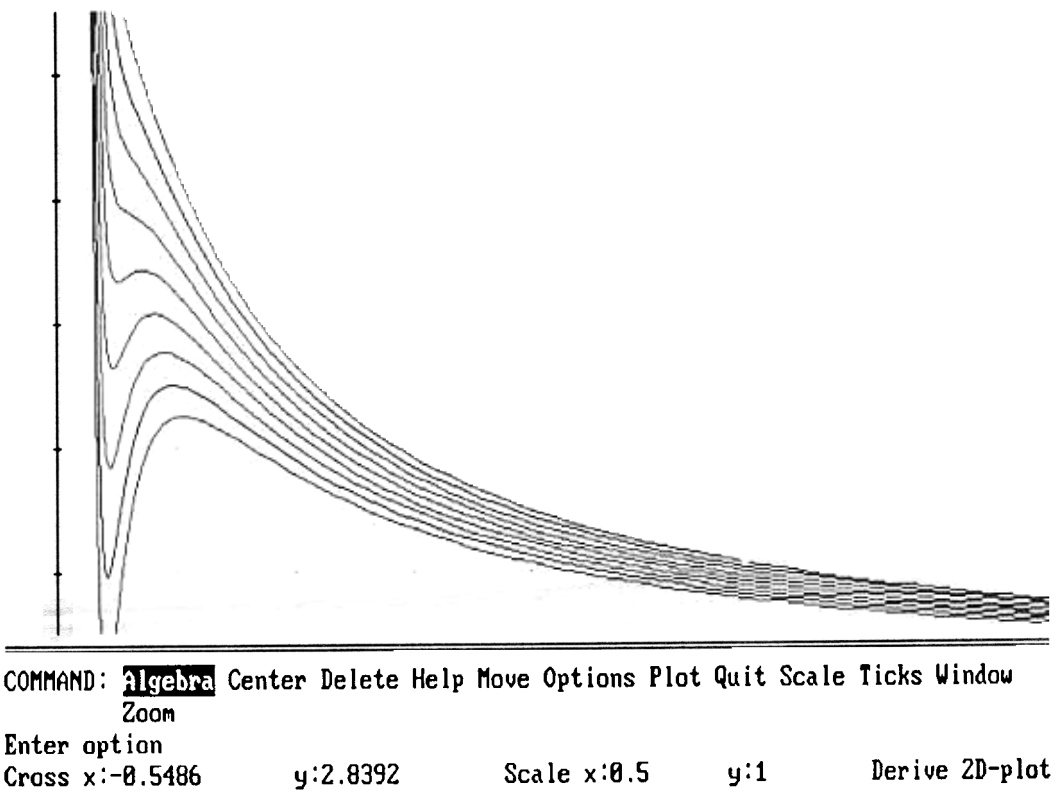


Fig. 3.2: isotherms (interval (t=2.5 , 3.3), step 0.1)

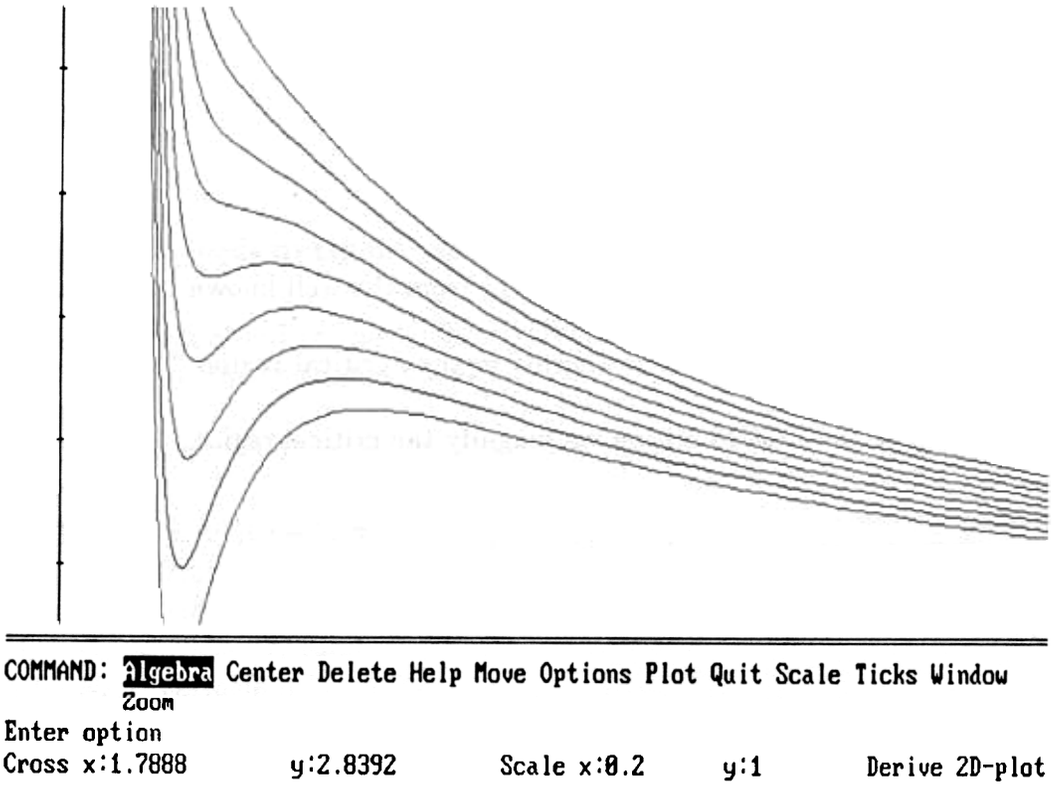


Fig. 3.3: Fig. 3.2 , using ZOOM option

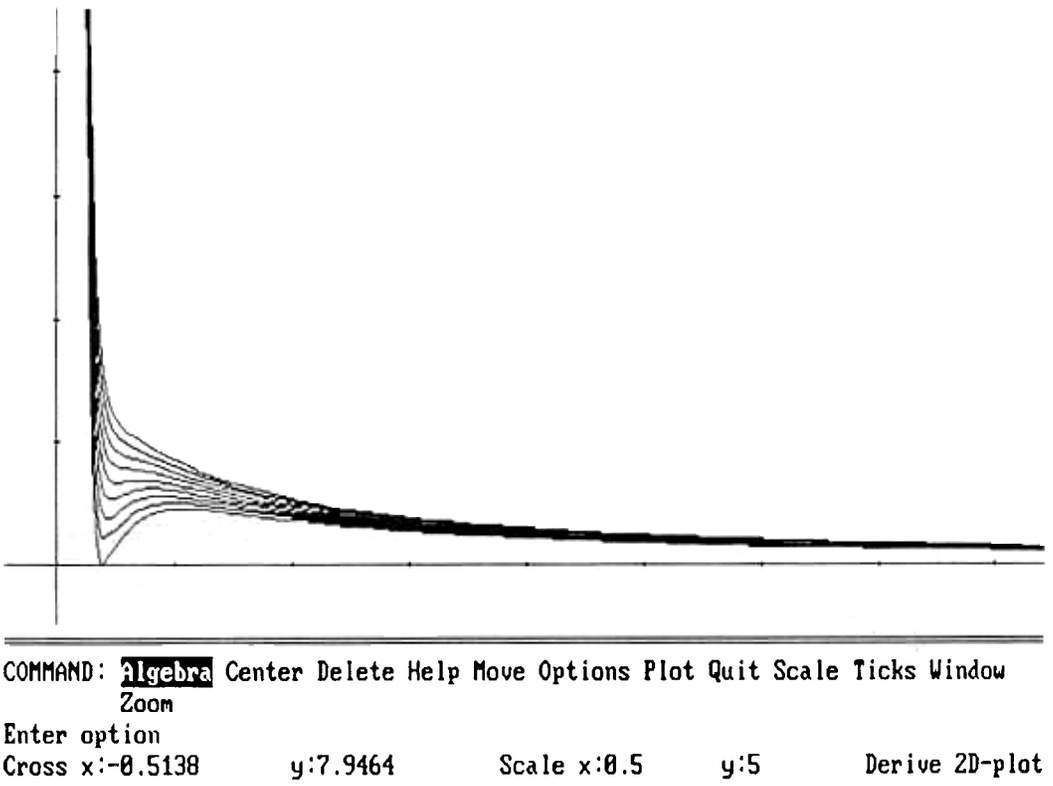


Fig. 3.4: Fig. 3.2 , different scaling of the y-axis (pressure)

physical interpretation of the plots

Fig. 3.4 shows a rapid rise in pressure in the left part of the isotherms. This means that any further decrease in volume is nearly impossible. We call this state "incompressible" or the "liquid state".
The maxima and minima of the isotherms are useless in our physical model. In this region our equation does not describe what is going on in the gas.
The isotherm with the horizontal tangent is a very special one, we call it "critical isotherm"("critical temperature").
Below the critical temperature the gas starts to condense from the vapor to the liquid phase. At temperatures greater than the critical temperature, no phase transition occurs as the material is compressed. With increasing temperature our real gas gets closer and closer to the ideal gas. (Fig. 3.5)

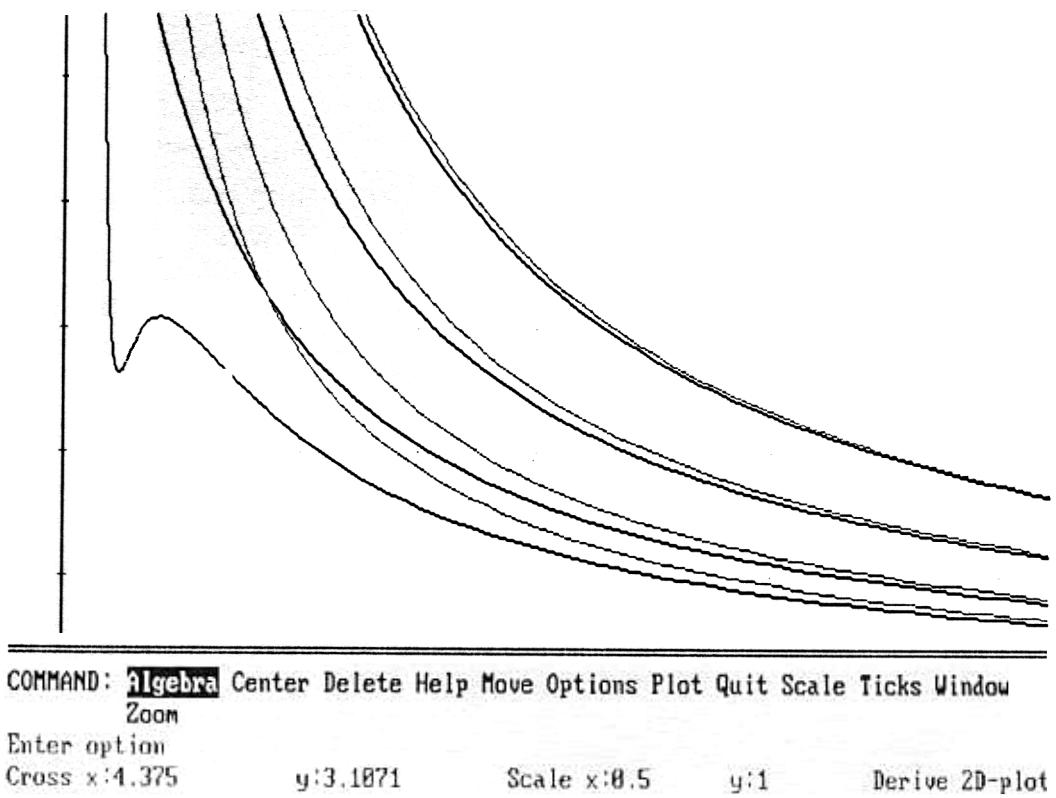


Fig. 3.5: isotherms of the real respectively ideal gas

4. Conclusions

We played the whole game only once, therefore it's too early to give you a complete report of experience.
There were no problems using DERIVE. The pupils did not even need the manual. All they need was one hour of training of the basic functions of DERIVE.
I think that their understanding of physics has been improved, but I'm not quite sure. Using DERIVE in the following years will show the improvements.
But doing gas dynamics in this way showed two clear results:

a) Most of the pupils had great fun doing gas dynamics.

b) The pupils asked more questions than the teacher.

In this sense, gas dynamics done with the help of DERIVE
was a success.