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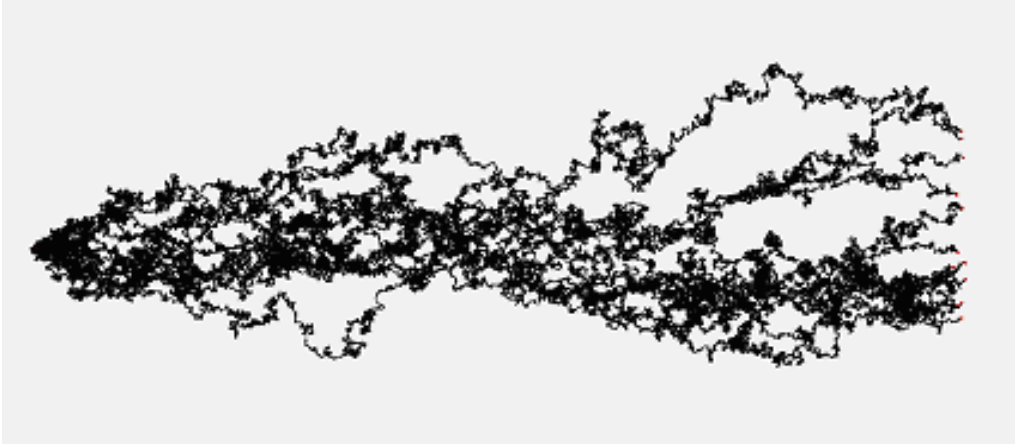
Simulation of ion movement in gas and related problems



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Introduction.

This report is part of scientific software 'Virtual Device v. 18'. The main goal of this report is developing model and algorithm of ion movement in supersonic jet. At present this report covers only model and algorithm of elastic ion collision in gas without supersonic jet. But later model of supersonic jet will be added to model of collisions. *Discussion of simulation of supersonic jet is part of Virtual Device with hydrodynamics.*

All research results referred to in the manual for this software belong to the author; reference is required.

Chapter 6. The tests for model of collisions (tests 1,2).

Our tests based on coefficient of mobility. **Test one:** calculation of coefficient mobility of Cs in nitrogen. Test presents itself a modeling of ion movement in resting gas, where ion placed between two parallel plates. Distance between plates 95 mm, 500 v applied between plates.

Test 1: The cross-section of Cs ion was taken from CRC hand book [16]. The numerical investigation was done in the following way. The coefficient of ion mobility can be expressed as [10]: $K = \frac{V_{dreif}}{E}$, where electrical field, V_{dreif} - velocity of ion under influence of electrical field. The electrical field is calculated by Simion software. Ion is moving in buffer gas under influence of electrical field through many collisions during some time Δt. During that time ion travels for some distance l. Therefore the drift velocity is l/Δt. Then ion mobility can be calculated according to the following formula: $K = \frac{l}{E \cdot \Delta t}$.

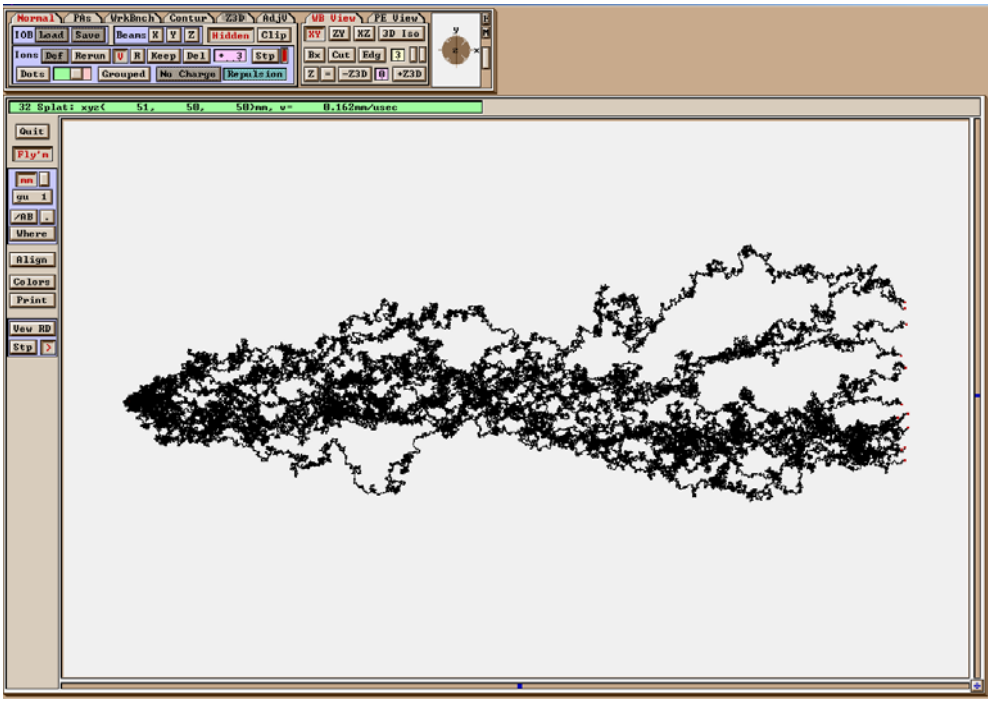
Initial parameters of simulation	Value
Mass of molecule of buffer gas	28 amu
Density of buffer gas (1 atmosphere)	$2.446 \cdot 10^{16}$ mm^3
Temperature of buffer gas	291 K
Distance	0.2 mm
Diameter of ion (Cs)	$489 \cdot 10^{-12}$ m
Energy of ion at start	1ev

Parameter 'distance' means length of ion movement. The results of simulation is following: Coefficient of mobility: 3.2 $sm^2/V•sec$. The experimental results of ion mobility is following [Mc Daniel., Mason E, 10]: 2.2 $sm^2/V•sec$. Actually this results is quite good but it is possible to get much better results. As it was mentioned above the main problem is in value of diameter of ion (cross-section of ion). Now we calculate the diameter of ion based on experimental results of ion mobility then we will use this diameter for our simulation, and at finely we will calculate the coefficient of ion mobility from our simulation. As it was mentioned above there is correlation between diameter of molecule and coefficient of mobility ($Z = 0.441 \cdot \frac{q \cdot (kT/m)^{1/2}}{Pd^2}$). Therefore if coefficient is 2.2 then diameter of Cs is $652•10^{-12}$m (charge 1).

Test 2. Simulation of Cs ion movement in nitrogen.

Initial parameters of simulation	Value
Mass of molecule of buffer gas	28 amu
Density of buffer gas (1 atmosphere)	$2.446•10^{16}$ mm^3
Temperature of buffer gas	291 K
Distance	0.2 mm
Diameter of ion (Cs)	$652•10^{-12}$ m
Energy	1ev

The results of our simulation is following: **Coefficient of mobility: 2.13 $sm^2/V•sec$.** As we can see we got quite well coincidence with experimental results.



Picture 2. Example of simulation of ion movement in SIMION.

Actually the pure Monte Carlo simulation is very time consuming. For example, to calculate 100 ion movement under parameters in previously tests it necessary about 50 hours (1 trajectory per 30 minutes). We used computer Pentium 4, 512 RAM). But there is a way to accelerate the simulation. Let us discuses it in following two chapters.

8.1. Tests 3, 4, 5 (big step algorithm).

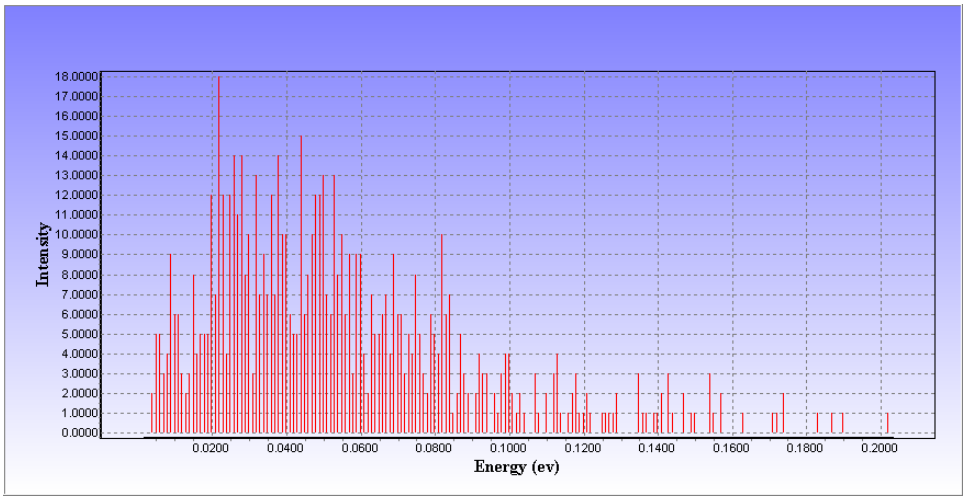
Test 3. Simulation of Cs ion movement in nitrogen (big step algorithm).

Initial parameters of simulation	Value
Mass of molecule of buffer gas	28 amu
Density of buffer gas (1 atmosphere)	$2.446 \cdot 10^{16}$ mm^3
Temperature of buffer gas	291 K
Distance	0.2 mm
Diameter of ion (Cs)	$652 \cdot 10^{-12}$ m
Energy	1ev

The results of simulation is following: **Coefficient of mobility: 2.3 sm^2/V•sec.**

But speed of calculation is about 1 trajectory per 2 minutes (Pentium 4, 2,8, 512 mb RAM). **Therefore our "Big step" algorithm works about 15 times faster then pure Monte-Carlo algorithm without loosing quality of calculation.** ***It is necessary to note that we did tests for ion movement in gas under normal condition (1 atmosphere). Therefore simulation of ion movement in region with lower pressure can be done very quickly. Actually this is typical way of simulation of ion movement in gas. Scientist use lower pressure to estimate ion mobility then this mobility can be transform to ion mobility under normal condition [10].***

Energy distribution of ions: When ions completely stopped by gas (in case of small value of electrical field therefore), energy distribution of ions has to be as Maxwell distribution. We used 500 volts in our tests. It close to weak field according to Mc Daniel [10], therefore energy distribution has to be close to Maxwell distribution. Picture 3 shows energy distribution of ions in test 3. This distribution is very similar to Maxwell distribution.



Picture 3. Energy distribution of ions in test 3.

Test 4. Coefficient of mobility can be also expressed as [10]. It is theoretical approach:

$$K_{pol} = \frac{e}{\mu V} = \frac{q}{\mu N g 2\pi \left(\frac{\alpha e^2}{\pi \varepsilon_0 \mu g^2} \right)^{\frac{1}{2}} \cdot 0{,}298} = \frac{\sqrt{\varepsilon_0}}{0{,}596 N \sqrt{\mu \pi \alpha}}$$

Below is table 1 representing the comparison of results of simulation based on model described above with results from theory[10]. We used small steps algorithm.

Table 1.

m, (amu)	μ, (amu)	E, V/sm	E/N, Taunsend	T, K	K_{exper}, $sm^2/V \cdot sec$	$K_{(pol)}$, $sm^2/V \cdot sec$	Ratio $K_{exper}/K_{(8)}$
10	7,4	670	2,5	0	7,20±0,23	7,14	1,01
				293	8,57±2,14		1,2
132	23,1	3,3	0,0013	0	4,16±0,01	4,031	1,03
		670	2,5	0	4,07±0,07		1,01
				293	4,28±0,73		1,06
				1000	4,98±1,38		1,24
		3300	12,3	293	4,17±0,57		1,03
		6700	24,8	0	4,05±0,18		1,005
				293	4,03±0,24		1,0
		33000	124	0	3,95±0,30		0,98
				293	3,95±0,32		0,98
		133000	496	0	3,70±0,46		0,92
				293	3,71±0,51		0,92
1320	27,4	670	2,5	0	3,78±0,06	3,7	1,02
				293	3,84±0,61		1,03

E – intensity of electrical field, E/N – parameter in term of Taunsend, [1 Td]=[10^{17} V·sm^2], T – temperature, m – mass of ion, μ - relative mass of ion and molecule, K_{exper} – coefficient of mobility got from numerical experiment, $K_{(pol)}$ – coefficient of mobility calculated according last formula.

The numerical investigation was done in the following way. The coefficient of ion mobility can be expressed as [10]: $K = \frac{V_{dreif}}{E}$, where electrical field, V_{dreif} - velocity of ion under influence of electrical field. The electrical field is calculated by Simion software. Ion is moving in buffer gas under influence of electrical field through many collisions during some time Δt. During that time ion travels for some distance l. Therefore the drift velocity is l/Δt. Then ion mobility can be calculated according to the following formula: $K = \frac{l}{E \cdot \Delta t}$. Table 1 above presents the comparison of numerical calculation and results calculated from last formula.

Test 5. Coefficient of diffusion can be expressed as [10]: $D = \frac{kT}{q} K$

Table 2.

m, amu	D_{exper}, см^2/с	$D_{(9)}$, см^2/с	Ratio D_{exper}/ $D_{(9)}$
10	0,18	0,18	1,0
132	0,1	0,102	0,98
1320	0,089	0,093	0,96

m – mass, D_{exper} – coefficient is calculated from numerical simulation, $D_{(9)}$ – coefficient is calculated according to last formula.

The algorithm of numerical calculation: diffusion coefficient is calculated according to algorithm of calculation of coefficient of mobility.

The comparison of results gotten from numerical simulation and from theory show that the model of collisions described is valid for case of ion traveling in buffer gas under influence of the electrical field. But there is a difference between theoretical and real experimental results. The experiment gives coefficient of mobility/diffusion smaller than coefficient from theory/numerical model.

The main problem again arises from estimation of cross-section. Let us discuss it again. We will calculate the cross-section according to coefficient of diffusion gotten from experiment. Then we will use this cross-section in numerical simulation to get coefficient of diffusion. We can compare results of calculation of diffusion coefficient with the coefficient received in the experiment.

In the case of weak field, the time between collisions is $\tau = (VN\sigma)^{-1}$, where $V = \left(\frac{3kT}{\mu}\right)^{\frac{1}{2}}$ - relative velocity, N – dencity, $2{,}69 \cdot 10^{19}$ sm^{-3}, σ - cross-section. Then , if m>>M, cross-section can be expressed in the terms of coefficient of diffusion, and temperature[10]: $\sigma = 0{,}47 \frac{(kT)^{3/2}}{DpM^{1/2}}$, where p – pressure ($1{,}013 \cdot 10^5$ Pa) , T – temperature (293 K), N=$2{,}5 \cdot 10^{19}$sm^{-3}.

Coefficients of diffusion (from real experiment):

1. $D_{N_2}^{Cs^+} = 0.051\,\text{sm}^2/\text{sec}$

2. $D_{N_2}^{Rb^+} = 0.053\ \text{sm}^2/\text{sec}$

Therefore cross-section will be:

$\sigma_{N_2}^{Cs^+} = 1{,}085 \cdot 10^{-12}\,\text{mm}^2$,

$\sigma_{N_2}^{Rb^+} = 1{,}044 \cdot 10^{-12}\ \text{mm}^2$.

Those cross-sections were used in numerical experiments to calculate the coefficients of diffusion and mobility. The results are presented in table 3 below.

Table 3.

ion	D_{numer}, sm^2/sec	D_{exper} sm^2/sec	Ratio D_{numer}/ D_{exper}	K_{numer}, $sm^2/V\cdot sec$	K_{exper}[22], $sm^2/V\cdot sec$	Ratio K_{numer}/ K_{exper}
Cs^+	0.063	0.051	1.24	2.68	2.36	1.14
Rb^+	0.07	0.053	1.32	2.96	2.40	1.23

This table shows that if cross-section is calculated from experiment, numerical simulation based on theory gives correct results.

Conclusion: The numerical model of ion movement described above gives results which coincide well with results (coefficient of diffusion and mobility) gotten from theory. But those results slightly differ from experiment. The main problem is in calculation of value of cross-section. If the cross-section can be calculated from experiment and then used in numerical model, then our numerical model gives correct results (well coincidence with experiments). The value of cross-section can be calculated from data on mobility, but those data don't cover the full mass range 315-$4.03\cdot10^{11}$ amu.