Санкт-Петербургский
государственный
университет
www.spbu.ru

SOFTWARE PRODUCT DEVELOPMENTFOR MODELING THE CHEMICAL GAS RELAXATION BEHIND A SHOCK WAVE

ВВЕДЕНИЕ

For modeling of gas relaxations, proprietary closed-source software is currently used. The purpose of this work is to implement a software package based on open-source libraries

ТЕОРИЯ

Let's write out a system of equations:

$$v\frac{\mathrm{d}n_{O_2}}{\mathrm{d}x} + n_{O_2}\frac{\mathrm{d}v}{\mathrm{d}x} = R_{O_2}^{\mathrm{react}(0)},$$

$$v\frac{\mathrm{d}n_{O}}{\mathrm{d}x} + n_{O}\frac{\mathrm{d}v}{\mathrm{d}x} = R_{O}^{\mathrm{react}(0)},$$

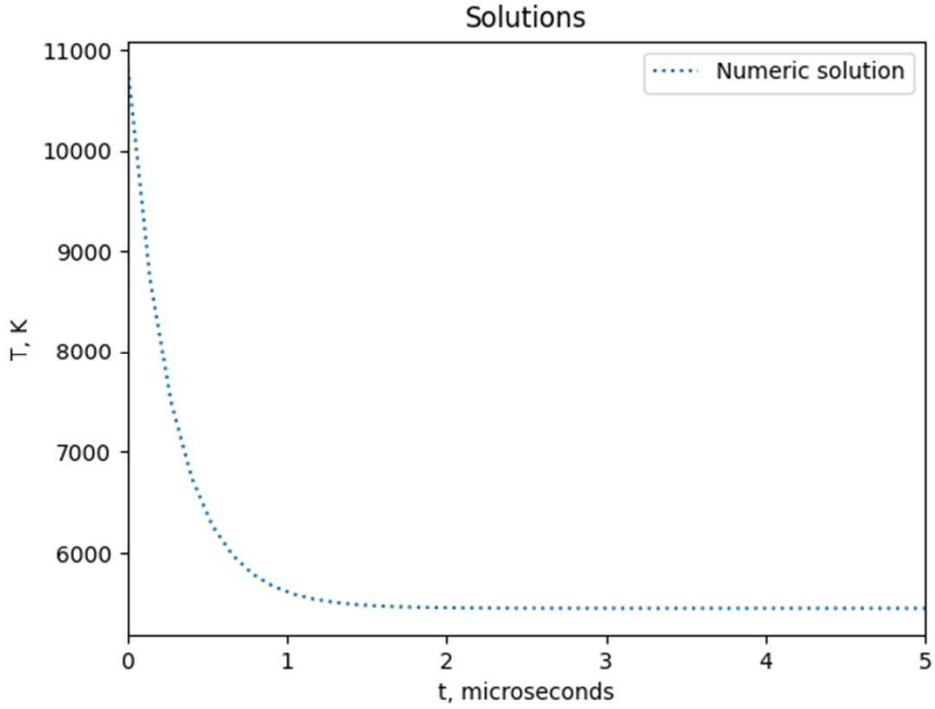
$$(m_O n_O + m_{O_2} n_{O_2})v\frac{\mathrm{d}v}{\mathrm{d}x} + kT\frac{\mathrm{d}n_O}{\mathrm{d}x} + kT\frac{\mathrm{d}n_{O_2}}{\mathrm{d}x} + (n_O + n_{O_2})k\frac{\mathrm{d}T}{\mathrm{d}x} = 0,$$

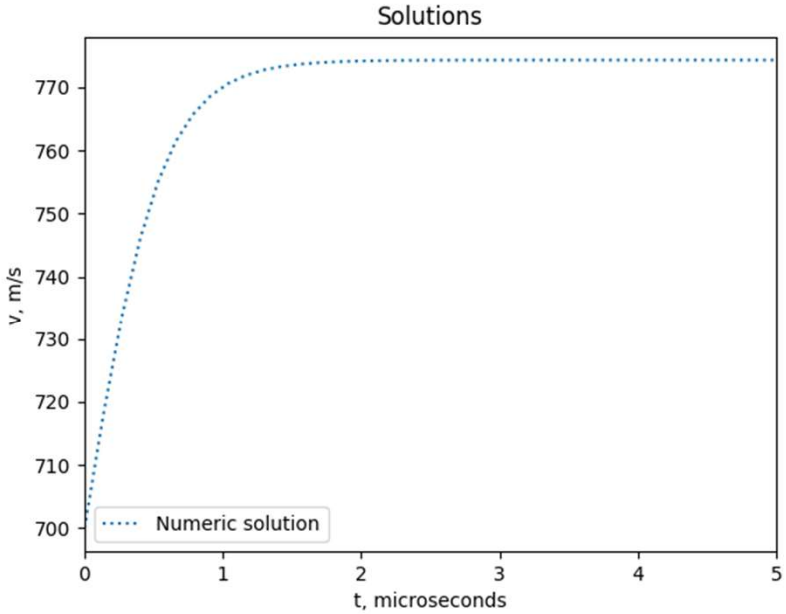
$$\rho v\frac{\mathrm{d}U}{\mathrm{d}x} + (n_{O_2} + n_O)kT\frac{\mathrm{d}v}{\mathrm{d}x} = 0,$$

Computation pipeline

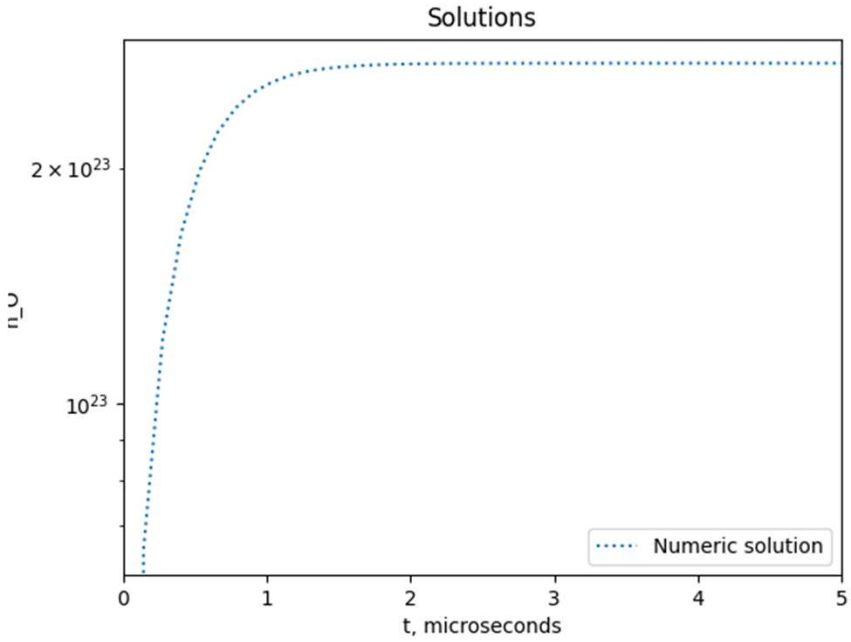
```
# Main loop
for i in range(0, N):
    dump_intermediate_data()
    x = solve_linear_system(n_O, n_O2, v, T, R_O, R_O2)
    if x[0] * x[1] >= 0 or np.abs(x[3]) < eps:
        break
    t_space, res = solve_eq(
        lambda t, Y: x,
        [n_O, n_O2, v, T],
        "RK45",
        accuracy, i)

    n_O, n_O2, v, T = res
    k_O_diss, k_O2_diss = calc_k(n_O, n_O2, v, T)
    R_O, R_O2 = calc_R(n_O, n_O2, v, T, k_O_diss, k_O2_diss)
```

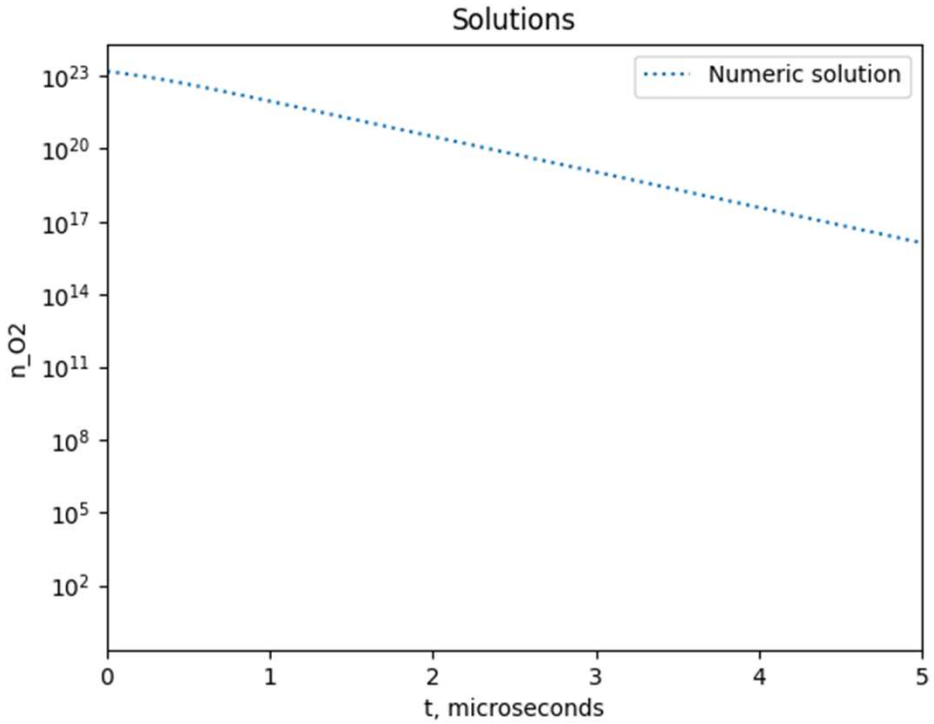
РЕЗУЛЬТАТЫ


Solutions
Numeric solution
T, K
t, microseconds
11000
10000
9000
8000
7000
6000
0
1
2
3
4
5


Solutions
Numeric solution
v, m/s
t, microseconds
770
760
750
740
730
720
710
700
0
1
2
3
4
5

РЕЗУЛЬТАТЫ


Solutions
2×10^{23}
10^{23}
n_O
Numeric solution
0
1
2
3
4
5
t, microseconds


Solutions
10^{23}
10^{20}
10^{17}
10^{14}
10^{11}
10^{8}
10^{5}
10^{2}
n_O2
Numeric solution
0
1
2
3
4
5
t, microseconds

РЕЗУЛЬТАТЫ

Computing time

```
chansons@chansons: ~/Reposito  ×  chansons@chansons: ~/Repo:  ×  chansons@chansons: ~  ×  +
chansons@chansons:~/Repositories/hydroaeromech/O2_O/solution$ time ./ex.py -b 0 -e 1 -a 1e-6
14699

real    0m4.855s
user    0m5.365s
sys     0m1.925s
chansons@chansons:~/Repositories/hydroaeromech/O2_O/solution$ time ./ex.py -b 0 -e 1 -a 1e-7
147198

real    0m35.275s
user    0m35.482s
sys     0m2.228s
chansons@chansons:~/Repositories/hydroaeromech/O2_O/solution$ time ./ex.py -b 0 -e 1 -a 1e-8
1472181

real    5m25.106s
user    5m24.642s
sys     0m2.875s
```

ЗАКЛЮЧЕНИЕ

- The problem of gas modeling in the one-temperature approximation is solved
- A physically based solution is obtained
- MVP developed

In the future: KAPPA integration, calculation in level approximation, comparison with experiment, support for universal mixtures and initial conditions


Санкт-Петербургский
государственный университет
spbu.ru