Breakdown voltage calculations using PIC-DSMC

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Motivation for understanding electrical breakdown mechanisms

"Undesired or unintended electric arcing can have detrimental effects on electric power transmission, distribution systems and electronic equipment. Devices which may cause arcing include switches, circuit breakers, relay contacts, fuses and poor cable terminations." Source: http://en.wikipedia.org/wiki/Electric_arc

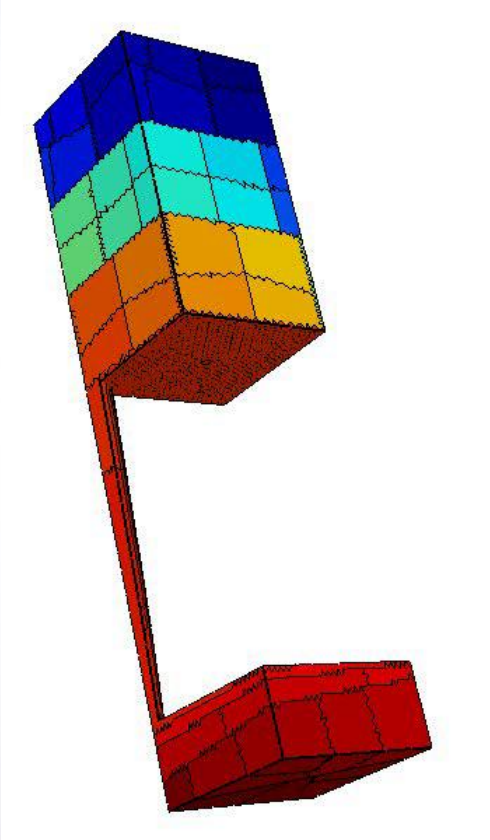
Motivation for computing breakdown voltages using PIC-DSMC

- Enable predictions of breakdown voltages as a function of gas composition, pressure, device geometry, and imposed E fields.
- Yield a better physical understanding of breakdown phenomena.
- Provide tests for simulation software: compute breakdown voltages and perform code-to-code verification exercises.
- Provide tests for models (interaction cross-sections, interaction models), which can be validated versus experimental measurements.
- Provide tests for theory (i.e. illustrate cases where Paschen equation assumptions are not valid).

"Electrical breakdown occurs within a gas (or mixture of gases, such as air) when the dielectric strength of the gas(es) is exceeded."

Source: http://en.wikipedia.org/wiki/Electrical_breakdown

Brief overview of the *Aleph* code



- Hybrid PIC + DSMC
- Electrostatics
- Fixed B field
- Conduction
- Ambipolar approximation
- Dual mesh (Particle and Electrostatics/Output)
- Advanced surface (electrode) physics models
- Collisions, charge exchange, chemistry, ionization
- Advanced particle weighting methods
- Unstructured FEM (compatible with CAD)
- Massively parallel
- Dynamic load balancing (tricky)
- Restart (with all particles)
- Agile software infrastructure for easily extending BCs, post-processed quantities, etc.
- Uses elements of SIERRA, Trilinos and other Sandia investments
- Currently utilizing up to 8192 processors (>30M elements, >1B particles)

Goals

1. Use *Aleph* to produce breakdown voltage curves for N_2.
2. Verify *Aleph* results vs BOLSIG+ (an electron-boltzmann equation solver).
3. Ensure that 2D/3D simulations can likewise be used to produce the same results.
4. Provide starting point input and procedures for complex 2D/3D geometry breakdown simulations.

How to get breakdown voltage from a PIC-DSMC simulation

Option 1

1. 0D (or higher) simulation, constant E field.
2. Use a stationary gas and no ions.
3. Reach a steady state condition for the electrons.
4. Compute steady state ionization coefficient.
5. Use Paschen's equation to deduce breakdown voltage (V_b).

Option 2

1. 1D (or higher) simulation.
2. Include mobile gas, ions, electrodes, and secondary emission.
3. Track gap current and wait for avalanche.
4. Run multiple simulations, varying gap voltage.
5. Converge on V_b at the boundary between voltages that lead to breakdown and those that don't.

Paschen's law

Γ_e= electron flux
Γ_i= ion flux
α = 1st Townsend coefficient (inverse of ionization mean free path)

1. Write a differential equation for the increase in electron flux as we move towards the anode.

$$d\Gamma_e = \alpha(z)\, \Gamma_e dz$$

2. Integrate.

$$\Gamma_e(z) = \Gamma_e(0) \exp \int \alpha(z')dz'$$

3. Assume that the field (E), the electron drift velocity (μ), and α are all constant (spatially invariant).

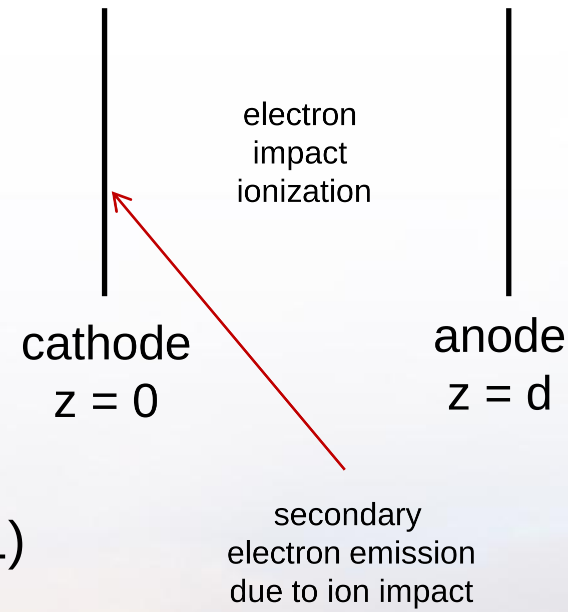
$$\Gamma_e(d) = \Gamma_e(0) \exp(\alpha d)$$

4. By continuity of total charge, and since bulk ion creation equals bulk electron creation.

$$\Gamma_i(0) - \Gamma_i(d) = \Gamma_e(d) - \Gamma_e(0)$$

5. Substituting.

$$\Gamma_i(0) - \Gamma_i(d) = \Gamma_e(0)\, (\exp(\alpha d) - 1)$$

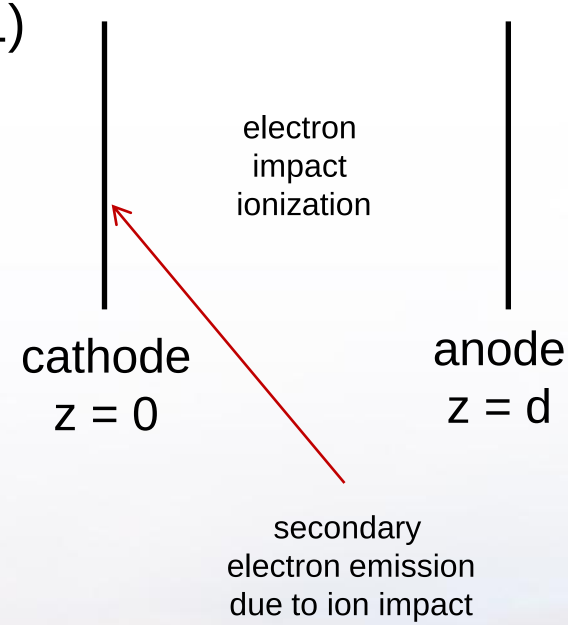


Major assumptions:
1. 1D
2. E and α constant

Paschen's law (continued)

γ_{se} = 2nd Townsend coefficient (electrons produced per ion impact at the cathode)
λ_e = mean free path for inelastic electron collisions
ε_{iz} = energy for ionization

1. (From last slide.) $$\Gamma_i(0) - \Gamma_i(d) = \Gamma_e(0)\,(\exp(\alpha d) - 1)$$
2. Electrons produced at cathode due to ion impact only. $$\Gamma_e(0) = \gamma_{se}\,\Gamma_i(0)$$
3. No ion flux at the anode. $$\Gamma_i(d) = 0$$
4. Substituting and rearranging. $$\alpha d = \ln\left(1 + \frac{1}{\gamma_{se}}\right)$$
5. We expect α to be expressed in this form. $$\alpha = \frac{const}{\lambda_e}\exp\left(-\frac{\varepsilon_{iz}}{E\lambda_e}\right)$$
6. λ_e proportional to the inverse of the gas pressure, $\lambda_e \propto \frac{1}{p}$ $$\frac{\alpha}{p} = A\exp\left(-\frac{Bp}{E}\right)$$

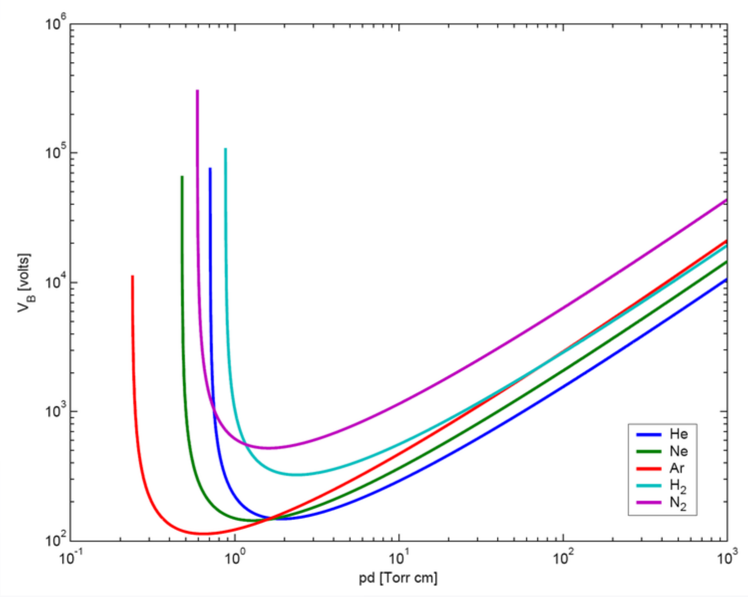


Major assumptions:

3. Electrons produced at cathode due to ion impact only.
4. A and B coefficients constant.

Paschen's law (continued)

V_b = breakdown voltage



1. (From last slide.)

$$\frac{\alpha}{p} = A\exp\left(-\frac{Bp}{E}\right)$$

2. (From last slide.)

$$\alpha d = \ln\left(1 + \frac{1}{\gamma_{se}}\right)$$

3. Combining the above, rearranging, and setting $V_b = Ed$.

$$Apd\exp\left(-\frac{Bpd}{V_b}\right) = \ln\left(1 + \frac{1}{\gamma_{se}}\right)$$

4. Solving for V_b.

$$V_b = \frac{Bpd}{\ln(Apd) - \ln\left(\ln\left(1 + \frac{1}{\gamma_{se}}\right)\right)}$$

<u>Major assumptions:</u>

1. 1D
2. E and α constant
3. Electrons produced at cathode due to ion impact only.
4. A and B coefficients constant.

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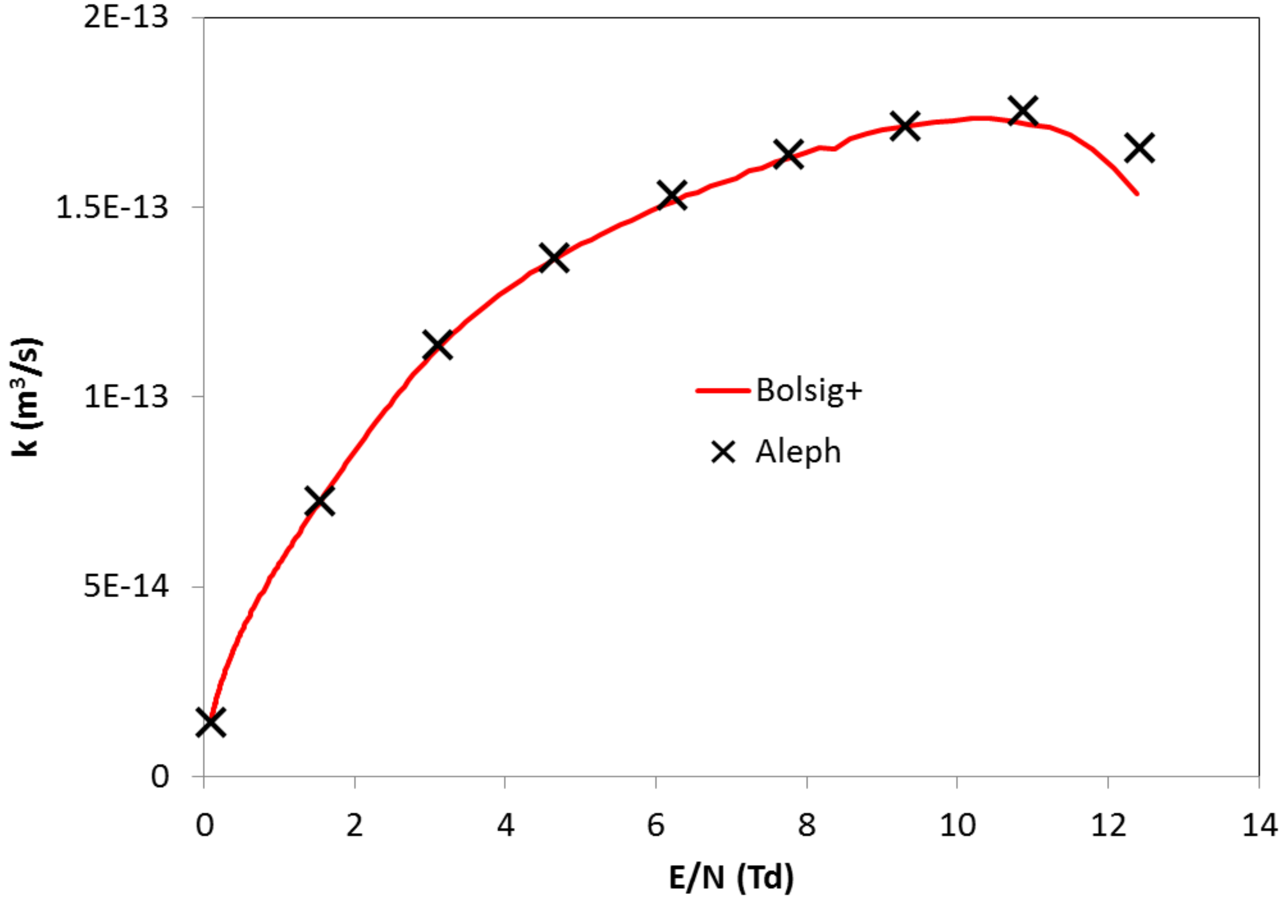
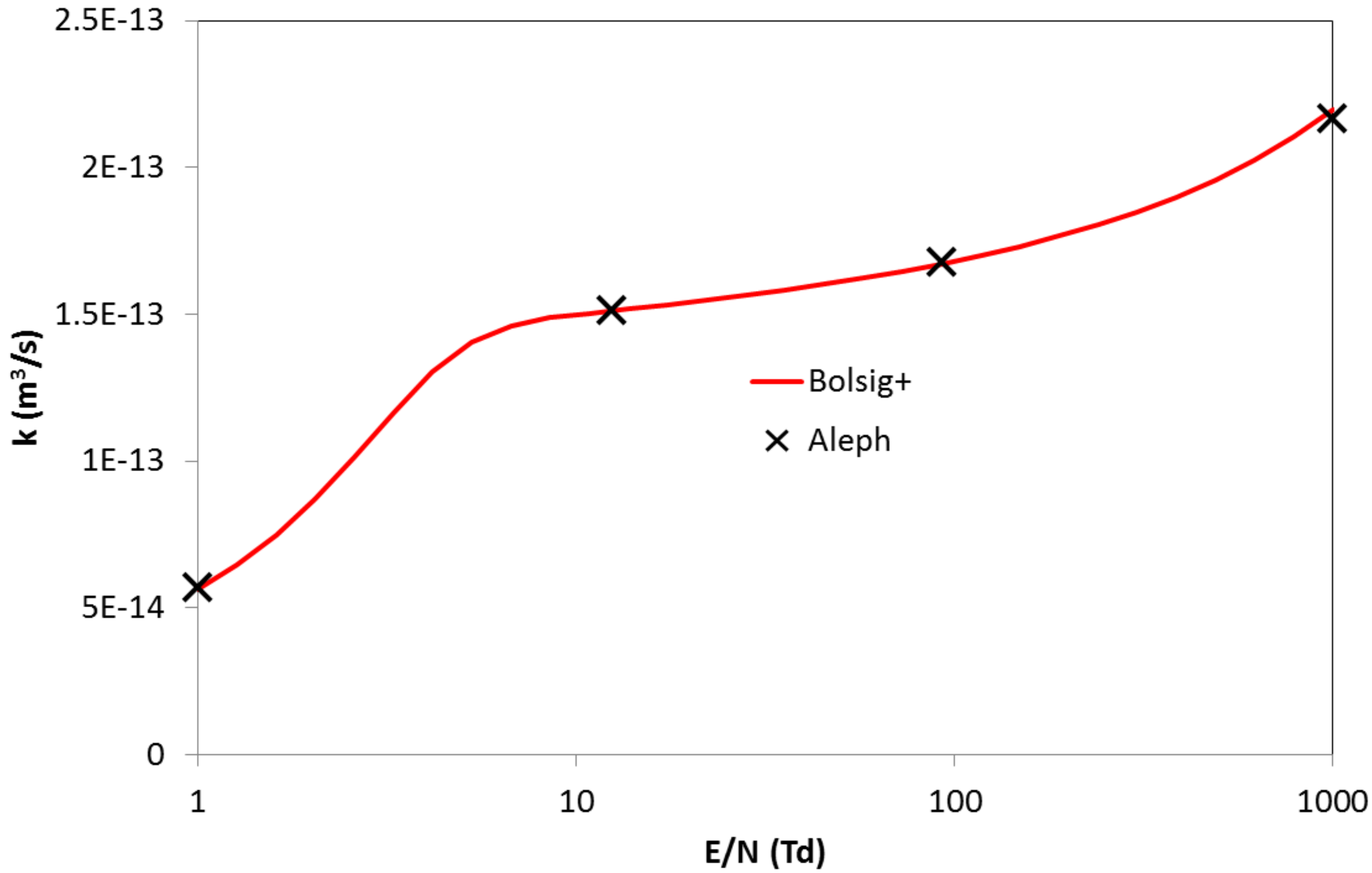
How to compute a Paschen curve using BOLSIG+ or *Aleph* ionization rate calculations

- **Input: α vs. E/N, γ**
  - α vs E/N can be computed from BOLSIG+ or *Aleph* given cross-section data.
  - γ can be set to a constant (depends on cathode material properties) as a reasonable approximation.
- **Output: V_b vs. pd (Paschen curve)**
- **Problem with Paschen's equation: A and B "constants" are not constant, but we can allow them to be variable functions of pd.**
- **We have a python script that takes the input (α vs. E/N from BOLSIG+ or Aleph) and fits this variable-coefficient version of Paschen's equation to produce the output (Paschen curve).**

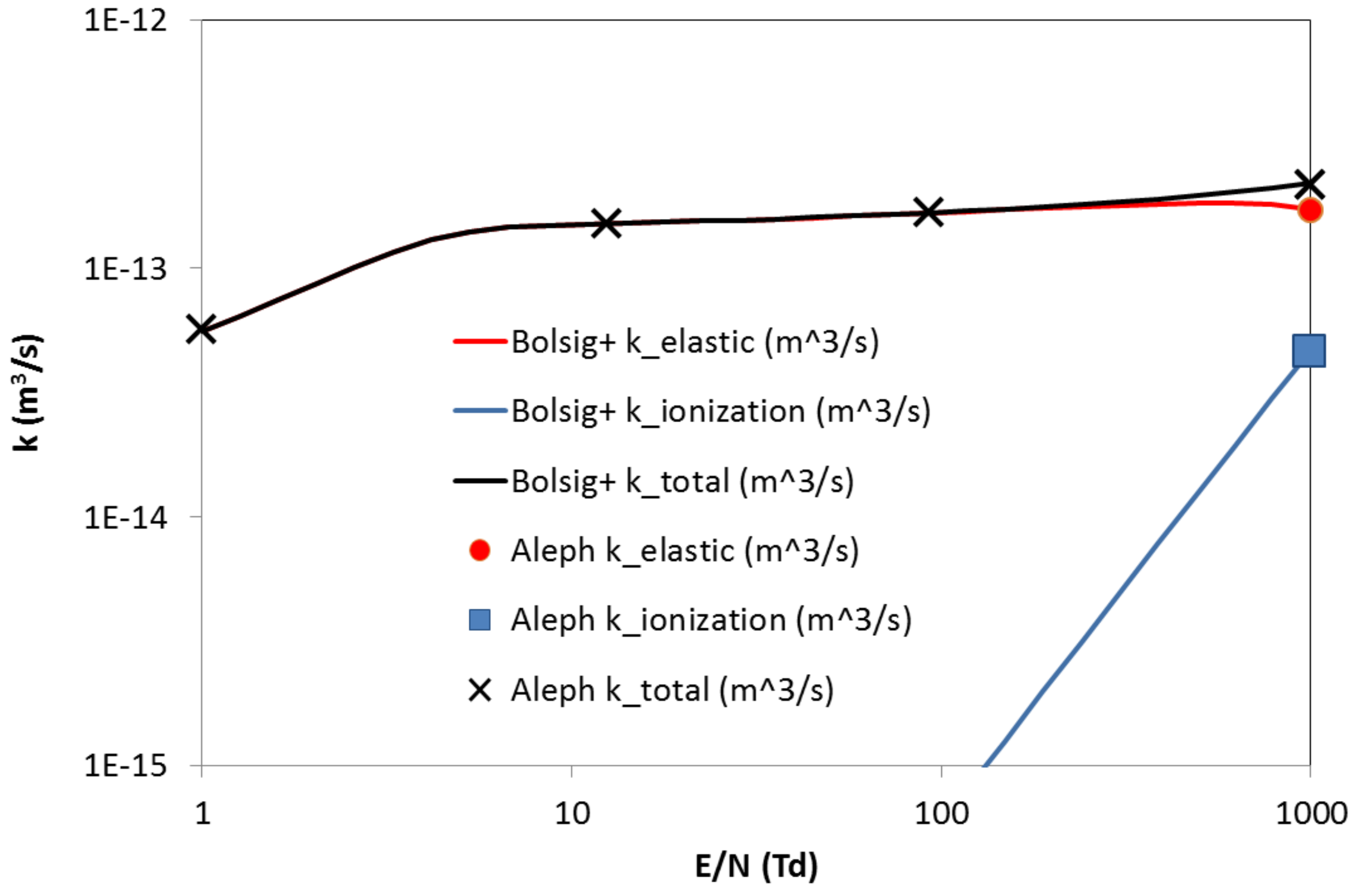
Aleph vs Bolsig+ elastic scatter rate constants for N2



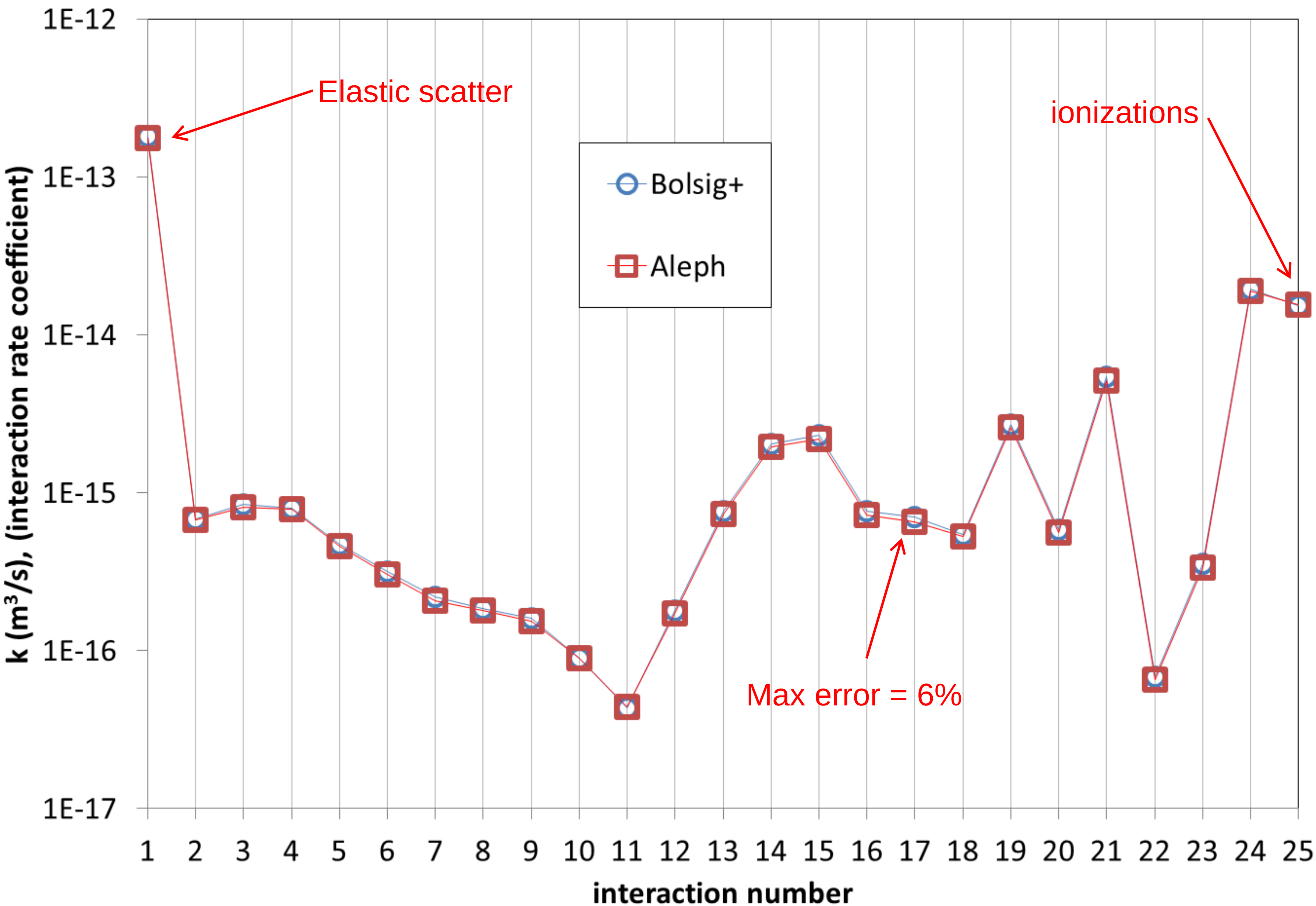
N_2 elastic scatter and ionizations



N_2 elastic scatter and ionizations



Now with all 25 interactions turned on, 1000 Td



To get good agreement between the codes, use the following settings:

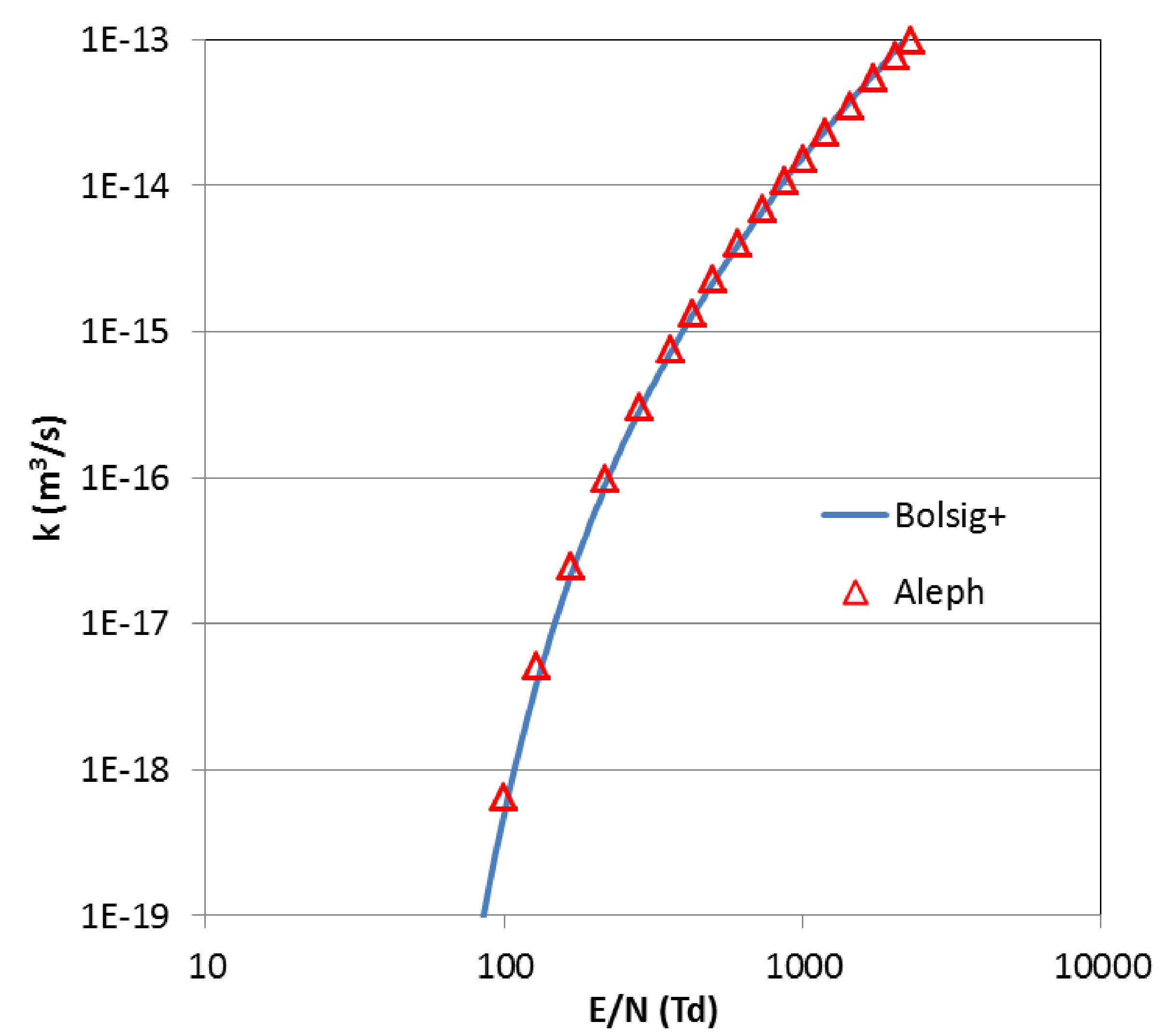
BOLSIG+

1. "Effect of electron production = Not included"
2. "Energy sharing after ionization = One electron takes all"
3. "Extrapolate cross sections" = off
4. # of grid points = 100
5. "Grid type = automatic"
6. Precision = 1e-10
7. Convergence = 1e-4
8. Max # of iterations = 1000

Aleph

1. quasi-0D mode: "particle position update = false"
2. "interaction_model = ionization" for all but elastic collisions.
3. "interaction_model = elastic_isotropic_scattering" for elastic collisions.
4. "fixed_heavy_particle_properties = true"

Aleph and Bolsig+ ionization rate coefficients



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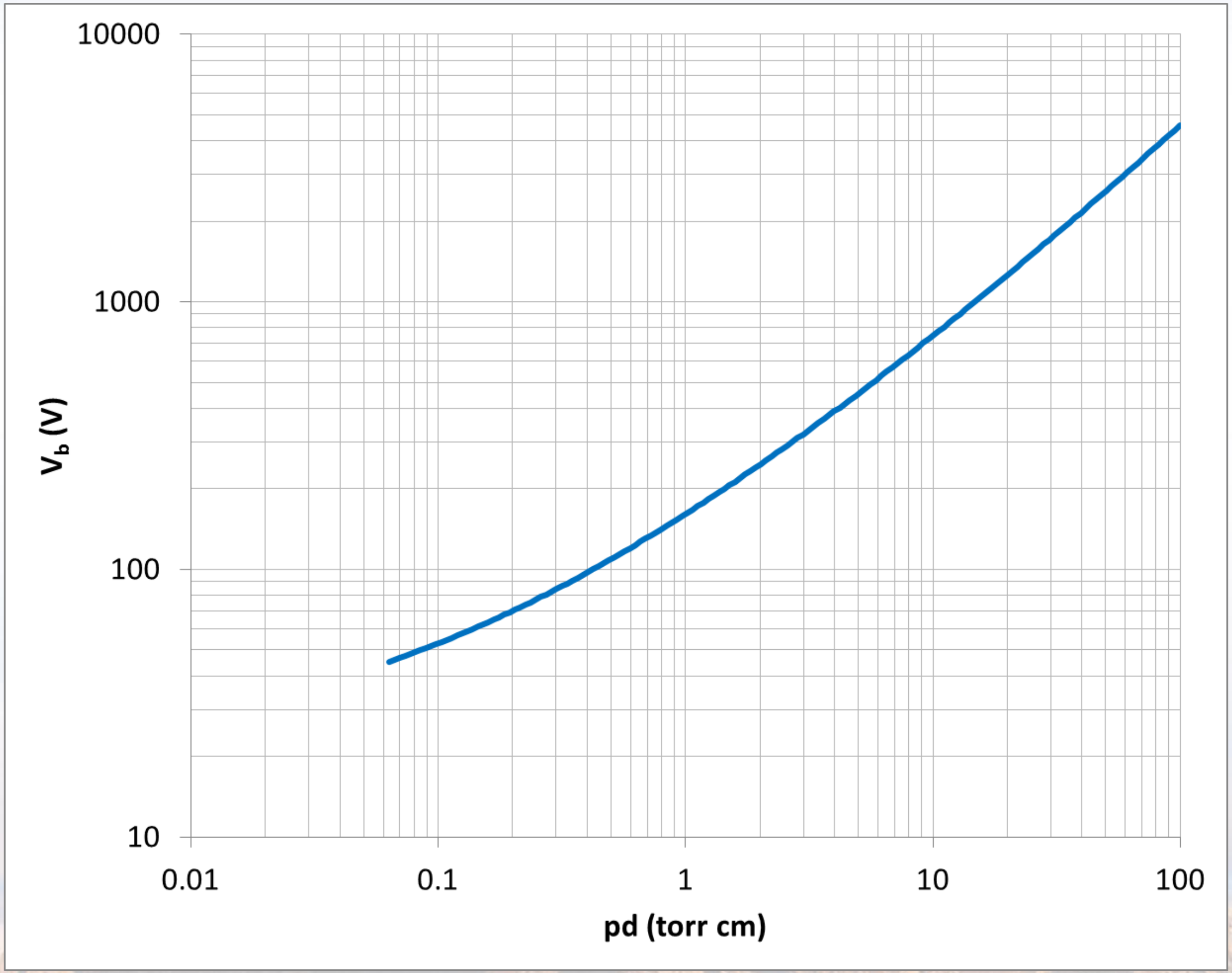
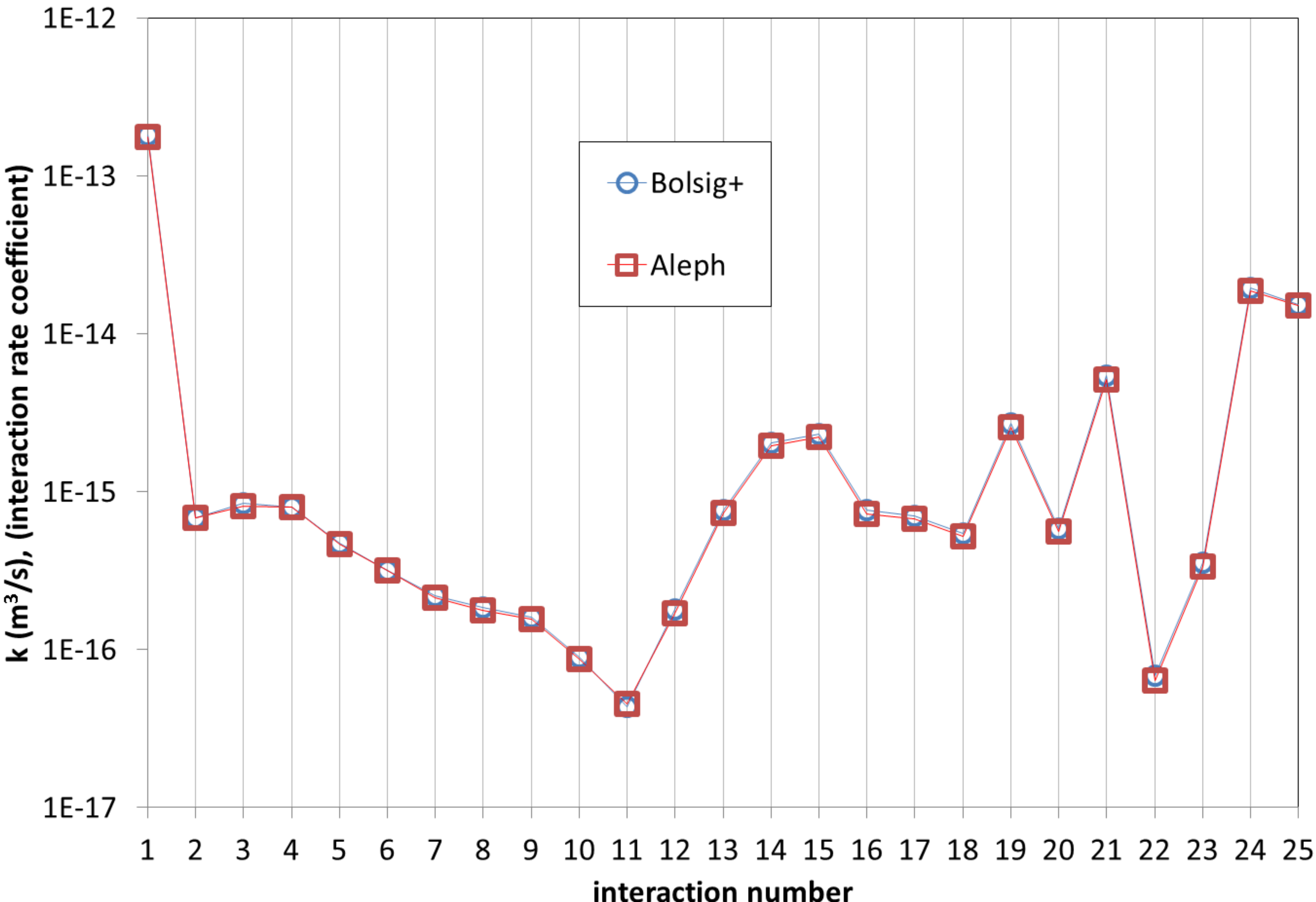
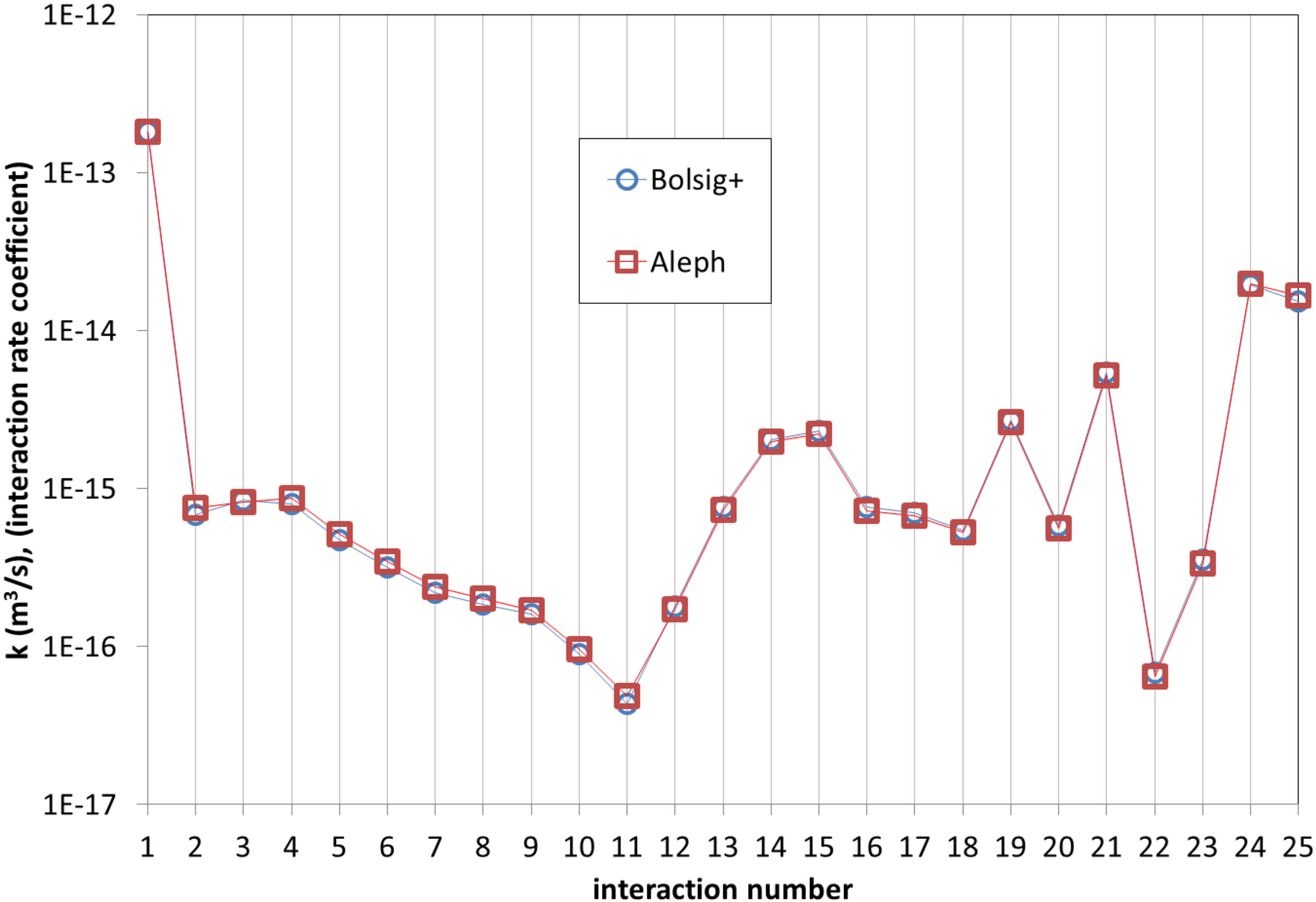
Bolsig+ model Paschen curve



3D, stationary particles



3D, dynamic particles



Summary and conclusions

- **Breakdown voltages computed using PIC-DSMC code (*Aleph*) agree well with BOLSIG+.**
- **Works in 3D geometry.**
- **Results can be extended to more difficult cases:**
  - Where experimental data unavailable.
  - Where Paschen's law assumptions are not valid, as in the cases of complex 3D geometries and microscale discharges.