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The **SIGLO**® series

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*Gas parameters and cross section data*

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**Note:** Any publications resulting from the use of this software should reference the SIGLO series of user friendly discharge modeling software.

# Gas parameter data for the SIGLO models

The software in the SIGLO series of discharge models all use the same format for the gas parameter data file, and library of gas parameter data, *gaspar.dat*, is provided with each of the SIGLO products. The structure of this data file and instructions for how to create data for gases and gas mixtures not in *gaspar.dat*, are described here.

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## What gas parameter data are provided with the SIGLO software?

The required data for each gas include the electron and ion (positive and negative) mobilities, the electron mean energy and the ionization (and attachment) rate as functions of E/p. The gas parameter data file provided with the SIGLO software contains data in the following 15 gases

He, Ne, Ar, Kr, Xe, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, CF<sub>4</sub>, SiH<sub>4</sub>, Cl<sub>2</sub>, F<sub>2</sub>, HCl, and SF<sub>6</sub>.

The electron mobilities, mean energy and ionization and attachment rates as functions of E/p which are compiled in *gaspar.dat* were calculated using a Monte Carlo simulation, and these results are shown graphically in figures at the end of this document. References for the cross section sets used in these calculations are given below. The Monte Carlo simulation is based on the algorithm of Boeuf and Marode (1982), but it simulates the transport and rate data in a Pulsed Townsend experiment. That is, the electron transport and rate data result from a spatially averaged, time dependent simulation. These calculated data are in reasonably good agreement with the available experimental data.

The positive and negative ion data are either taken from the literature or estimated. Specific references are provided below.

Note: Certain models in the SIGLO series (SIGLO-TR and SIPDP-2D) do not use the electron mean energy data. Nevertheless, for uniformity, it is in the gas parameter data file used by these models.

## Structure of the *gaspar.dat* file

The user can modify the *gaspar.dat* or include data for additional gases or gas mixtures by appending the additional data to *gaspar.dat*. For each gas and gas mixture used in the SIGLO models, a data set must be provided in the format shown in Tables A1 and A2.

There are several practical considerations to keep in mind when creating the data tables. First, if the optional data do not appear, they are set equal to zero. And second, we have found that it is especially important to include a large number of data points for the ionization rate as a function of E/p in the low E/p region where the ionization is a rapidly varying function of E/p. The SIGLO models use a linear interpolation to find values between those given in the tables, and numerical noise may be introduced by this interpolation procedure when the input data varies significantly between adjacent values in the table.

<b>1st line - gas name</b>	SIGLO-TR searches through the gas parameter data file for the gas name given as input in the conditions of the calculation. Therefore, it is essential to be consistent in the use of abbreviations for gas names.
<b>2nd line - nparticles, npos, nneg</b>	3 integers to specify a) the number of charged particles to be included in the calculation, b) the number of positive ions ( $\leq 2$ for SIGLO-rf, = 1 for other SIGLO models), and c) the number of negative ions ( $\leq 1$ )
<p><b>The following data tables MUST be present for each gas:</b> See Table A2 for the format of these data tables.</p> <p>If there is only one positive ion, these data may be given in any order. When two positive ion species are present, the data are identified with either the first or second ion species according to the order in which they appear in the data tables.</p>	
<b>electron mobility vs E/p</b> <b>positive ion mobility vs E/p</b> <b>mean electron energy vs E/p</b> <b>ionization coefficient vs E/p</b> <b>negative ion mobility vs E/p (if nneg <math>\neq</math> 0)</b> <b>attachment coefficient vs E/p (if nneg <math>\neq</math> 0)</b>	units of $\text{cm}^2 \text{ torr V}^{-1} \text{ s}^{-1}$ units of $\text{cm}^2 \text{ torr V}^{-1} \text{ s}^{-1}$ units of eV units of $\text{cm}^{-1} \text{ torr}^{-1}$ units of $\text{cm}^2 \text{ torr V}^{-1} \text{ s}^{-1}$ units of $\text{cm}^{-1} \text{ torr}^{-1}$
<p><b>The following OPTIONAL DATA TABLES may be present:</b> See Table A2 for the format of these data tables.</p> <p>The recombination and detachment loss terms, if present, must be immediately preceded by the corresponding ionization and attachment source terms.</p>	
<b>electron-ion recombination coefficient vs E/p</b> <b>ion-ion recombination coefficient vs E/p</b> <b>detachment coefficient vs E/p (if nneg <math>\neq</math> 0)</b>	units of $\text{cm}^3 \text{ s}^{-1}$ units of $\text{cm}^3 \text{ s}^{-1}$ units of $\text{s}^{-1}$
<p><b>last line of data set for a specific gas is indicated by:</b></p> <p><b>25 dashes: ‘-----’</b></p>	

Table A1. Structure of gas parameter data file

<b>1st line</b>	character string identifying by name the type of data to follow, with the identifying string being EXACTLY one of the following; <b>electron_mobility</b> <b>positive_ion_mobility</b> <b>negative_ion_mobility</b> <b>mean_electron_energy</b> <b>ionization_coefficient</b> <b>attachment_coefficient</b> <b>detachment_coefficient</b> <b>electron_ion_recombination_coefficient</b> <b>ion_ion_recombination_coefficient</b>
<b>2nd line</b>	<b>n</b> - number of entries in the data table = 1 if the data is independent of E/p
<b>Table of n values of E/p</b>	units of $V\text{ cm}^{-1}\text{ torr}^{-1}$ and at 300°K free format
<b>Table of n values of data</b>	immediately following the table of values of E/p, a table of data for the corresponding values of E/p in the units given in Table A1, free format

*Table A2. Format for electron and ion transport, mean electron energy and rate coefficient data tables. Any number of blank lines may appear between the data tables; SIGLO-TR searches for the character strings listed above for the 1st line.*

By way of example, we reproduce here the data for argon in *ingaspar.dat*.

	<b>Data in <i>ingaspar.dat</i></b>	<b>Comment</b>
Ar		Name of gas
2,1,0		Number of charged species = 2 Number of positive ions = 1 Number of negative ions = 0
electron_mobility [Monte Carlo simulation - see manual for cross-sections Refs]		string identifying data type
6		number of values of E/p
1.60900 3.21800 41.8400 138.400 241.400		table of values of E/p
376.500		
285800. 245300. 221400. 200000. 180300.		table of values of electron mobility
161500.		
positive_ion_mobility [Ar+ - Ar. H.W. Ellis et al., Atomic Data & Nucl Data Tab, 17,177 (1976)]		string identifying data type
29		number of values of E/p
2.57448 3.21810 3.86172 4.82715 6.43620		

8.04525	9.65430	12.8724	16.0905	19.3086
25.7448	32.1810	38.6172	48.2715	64.3620
80.4525	96.5430	128.724	160.905	193.086
257.448	321.810	386.172	482.715	643.620
700.000	800.000	900.000	1000.00	
1277.05	1277.05	1277.05	1268.71	1260.36
1243.67	1226.97	1201.93	1176.89	1151.85
1101.77	1060.04	1018.30	968.224	884.756
826.329	792.942	709.474	651.047	600.966
525.846	467.418	425.685	383.951	333.870
320.143	299.466	282.339	267.851	

table of values of E/p

table of values of mobility

mean\_electron\_energy [Monte Carlo simulation - see manual for cross-sections Refs]

55

1.60900	3.21800	4.82700	6.43600	8.04500
11.2600	14.4800	17.7000	22.5300	27.3500
32.1800	38.6200	45.0500	51.4900	57.9300
64.3600	74.0200	83.6700	93.3200	106.200
119.100	131.900	144.800	157.700	164.100
177.000	189.900	202.700	215.600	228.500
241.400	254.200	273.500	286.400	292.800
305.700	318.600	325.000	344.300	350.800
363.600	370.100	376.500	383.000	395.800
408.700	415.100	428.000	447.300	460.200
473.100	479.500	485.900	492.400	498.800
4.22800	5.15200	5.34800	5.48300	5.59800
5.78700	5.94200	6.07600	6.24900	6.40100
6.53900	6.71100	6.87200	7.02800	7.18000
7.33000	7.55200	7.77300	7.99600	8.24200
8.50600	8.82200	9.08500	9.32600	9.54200
9.80700	10.0800	10.3600	10.6000	10.9500
11.2600	11.5800	11.9600	12.2600	12.5900
12.8500	13.1700	13.4700	13.8500	14.2600
14.5700	14.7000	14.8000	15.1100	15.4400
15.9000	16.4400	17.1700	17.6600	18.2200
18.8600	19.0100	19.2400	19.6200	20.7500

ionization\_coefficient [Monte Carlo simulation - see manual for cross-sections Refs]

67

1.60900	3.21800	4.82700	6.43600	8.04500
9.65400	11.2600	12.8700	14.4800	16.0900
17.7000	19.3100	20.9200	22.5300	24.1400
25.7400	27.3500	28.9600	32.1800	35.4000
38.6200	41.8400	45.0500	48.2700	51.4900
54.7100	57.9300	61.1400	64.3600	67.5800
70.8000	74.0200	77.2300	80.4500	83.6700
86.8900	90.1100	93.3200	96.5400	99.7600
112.600	125.500	131.900	138.400	151.300
164.100	170.600	183.400	189.900	202.700
222.000	228.500	234.900	241.400	260.700
273.500	286.400	305.700	312.200	318.600
331.500	350.800	370.100	389.400	408.700
434.400	453.800			

0.000000	0.453100E-05	0.318300E-03	0.238600E-02	0.891700E-02
0.206200E-01	0.383100E-01	0.618100E-01	0.906200E-01	0.124000
0.161400	0.202100	0.245600	0.291300	0.338900
0.388100	0.438600	0.490200	0.595900	0.704100
0.814000	0.925000	1.03700	1.14900	1.26200
1.37400	1.48700	1.59900	1.71200	1.82400
1.93600	2.04700	2.15800	2.26900	2.38000
2.49000	2.59900	2.70800	2.81700	3.04300
3.39900	3.68700	4.12200	4.41400	4.67200
5.10100	5.42600	5.73000	6.18900	6.44200
6.94800	7.09200	7.34800	7.69600	8.30200
8.47000	8.83200	9.18900	9.41100	9.62800
10.0500	10.5700	11.0000	11.2900	11.6800
11.9600	12.5000			

## Creating data in other gases or gas mixtures

A convenient way to create data in gas mixtures is to use BOLSIG, the user friendly Boltzmann equation solver developed for the SIGLO series and distributed as shareware through ftp. Thus, BOLSIG calculates the electron mobility, mean energy and ionization rates as functions of E/p for a given gas mixture and over a range of values of E/p. A library of cross section data in He, Ne, Ar, Kr, Xe, H<sub>2</sub>, N<sub>2</sub>, O<sub>2</sub>, CH<sub>4</sub>, CF<sub>4</sub>, SiH<sub>4</sub>, Cl<sub>2</sub>, F<sub>2</sub>, HCl, and SF<sub>6</sub> is included with BOLSIG.

Running BOLSIG is easy - the menu guides the user through the running of the program. The user need only input the gas mixture and a table of values of E/p where the electron mobility, mean energy and rate coefficient data are to be calculated. BOLSIG creates a file which can be directly used by the SIGLO software.

Note: BOLSIG calculates only the electron data. The ion mobility data which is added to the file to make it compatible with the SIGLO models is a constant for all gases and all values of E/p. The user should edit this file and introduce more accurate data for the ion mobility if it is available.

## Structure of the cross section data file

BOLSIG reads the names of gases entered by the user and then searches through the cross section data file to find the data for those gases. The user may create or add to the cross section data file provided with BOLSIG. BOLSIG searches through the input data file for a line containing the word 'Species' starting in the first column. The character string on the next line is compared with the names of the gases input by the user. When there is an *exact match*, BOLSIG reads the cross section information. The format must be the same as in the example for argon shown below. Most of the notation will be obvious. For each collisional process, the number of entries in the cross section table, the threshold (energy loss), the maximum energy, the nature of the collision (NatCol) and a scale factor are given. The parameter 'NatCol' is set according to the following table.

NatCol = <b>0</b>	Elastic
= <b>1</b>	Inelastic
= <b>2</b>	Ionization
= <b>-1</b>	Attachment

### Example of input cross section data

### Comments (in italics)

Species  
Ar

*The word 'Species' appears on the line above the gas name.  
An exact match between the gas name on this line and  
the name in the input form is required.*

# of levels # excit # ioniz # attach  
5 3 1 0  
Mass Ratio m/M  
0.136000E-04

*Numbers of collisional processes of each type*

Momentum transfer (Hunter+Christophorou 1984 J.Chem.Phys.)  
elastic

*Blank line  
2-lines of comments and  
identifiers, free format*

# Points Threshold Max Ene NatCol Scale  
52 0.0000 1000.0000 0 1.0000

*(See paragraph above)*

-----  
0.0000E+00 0.1000E-01 0.1500E-01 0.2000E-01 0.3000E-01

*Table of values of energies (in eV)*

0.4000E-01 0.5000E-01 0.6000E-01 0.7000E-01 0.8000E-01  
0.9000E-01 0.1000E+00 0.1500E+00 0.2000E+00 0.3000E+00  
0.4000E+00 0.5000E+00 0.6000E+00 0.7000E+00 0.8000E+00  
0.9000E+00 0.1000E+01 0.1500E+01 0.2000E+01 0.3000E+01  
0.4000E+01 0.5000E+01 0.6000E+01 0.7000E+01 0.8000E+01  
0.9000E+01 0.1000E+02 0.1500E+02 0.2000E+02 0.3000E+02  
0.4000E+02 0.5000E+02 0.6000E+02 0.7000E+02 0.8000E+02  
0.9000E+02 0.1000E+03 0.1500E+03 0.2000E+03 0.3000E+03  
0.4000E+03 0.5000E+03 0.6000E+03 0.7000E+03 0.8000E+03  
0.9000E+03 0.1000E+04

*Free format*

0.7501E+01 0.4282E+01 0.3810E+01 0.3280E+01 0.2570E+01  
0.2050E+01 0.1662E+01 0.1357E+01 0.1114E+01 0.9160E+00  
0.7541E+00 0.6210E+00 0.2327E+00 0.1009E+00 0.1466E+00  
0.3169E+00 0.5040E+00 0.7044E+00 0.8788E+00 0.1050E+01  
0.1214E+01 0.1370E+01 0.2052E+01 0.2700E+01 0.4707E+01  
0.7143E+01 0.9412E+01 0.1227E+02 0.1519E+02 0.1740E+02  
0.1847E+02 0.1839E+02 0.1200E+02 0.8324E+01 0.5878E+01  
0.4877E+01 0.4228E+01 0.3394E+01 0.2886E+01 0.2678E+01  
0.2486E+01 0.2308E+01 0.1730E+01 0.1333E+01 0.8891E+00  
0.6273E+00 0.4671E+00 0.3665E+00 0.2980E+00 0.2485E+00  
0.2112E+00 0.1822E+00

*Blank line*  
*Table of values of corresponding*  
*cross sections (in units of  $10^{16}$  cm<sup>2</sup>).*  
*Free format*

*One blank line separates cross sections for different collisional processes*

*(For brevity, not all cross sections in argon are shown here )*

Rapp+Englander-Golden 1965 J.Chem.Phys  
IONIZATION Ar  
# Points Threshold Max Ene NatCol Scale  
20 15.7000 1000.0000 2 1.0000

*Two line description*

*NatCol=2, ionization*

-----  
0.1570E+02 0.1962E+02 0.2451E+02 0.3063E+02 0.3827E+02  
0.4782E+02 0.5975E+02 0.7465E+02 0.9328E+02 0.1166E+03  
0.1456E+03 0.1820E+03 0.2274E+03 0.2841E+03 0.3550E+03  
0.4435E+03 0.5542E+03 0.6925E+03 0.8652E+03 0.1081E+04

*Table of energies*

0.0000E+00 0.9007E+00 0.1730E+01 0.2338E+01 0.2810E+01  
0.3067E+01 0.3154E+01 0.3100E+01 0.2957E+01 0.2755E+01  
0.2515E+01 0.2263E+01 0.2011E+01 0.1768E+01 0.1542E+01  
0.1335E+01 0.1148E+01 0.9824E+00 0.8368E+00 0.7098E+00

*Table of cross sections*

## Electron scattering cross sections and ion mobilities

References to the cross section sets used in the Monte Carlo simulation for the electron transport, mean energy and rate coefficient and references for the ion transport, recombination and detachment data are given in this section. Unless otherwise specified below, the electron-ion and ion-ion recombination rates and the detachment frequency are taken to be zero.

N<sub>2</sub>:

The electron mobility, mean energy and ionization coefficient were calculated using the cross sections of Phelps and Pitchford (1985). The positive ion mobility as a function of E/p is that of N<sub>2</sub><sup>+</sup> in N<sub>2</sub> and the values are from Ellis et al (1976).

O<sub>2</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections of Phelps (1985). The positive ion mobility as a function of E/p is that of O<sub>2</sub><sup>+</sup> in O<sub>2</sub>, the negative ion mobility corresponds to O<sup>-</sup> in O<sub>2</sub>, and the values are from Ellis et al (1976). The ion-ion recombination rate is 10<sup>-7</sup> cm<sup>3</sup> s<sup>-1</sup> (Raizer, 1991).

H<sub>2</sub>:

The electron mobility, mean energy and ionization coefficient were calculated the cross sections of Buckman and Phelps (1985). The positive ion mobility as a function of E/p is that of H<sub>3</sub><sup>+</sup> in H<sub>2</sub> and the values are from Ellis et al (1976). No negative ions are included.

Cl<sub>2</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated the cross sections of Rogoff, Kramer and Piejak (1986). The positive and negative ion mobilities and constant and given by Park and Economou (1991). The ion-ion recombination is taken from Park and Economou (1991).

F<sub>2</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections compiled by Morgan (1992). The positive and negative ion mobilities are our estimates, and the ion-ion recombination rate is estimated by analogy with Cl<sub>2</sub>.

HCl:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections compiled by Morgan (1992). The positive and negative ion mobilities are constant and taken from Davies (1982). The ion-ion recombination is assumed to be  $2.10^7 \text{ cm}^3 \text{ s}^{-1}$ .

CF<sub>4</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections of Nakamura (1991). The positive and negative ion mobilities are constant and taken from Kono (1991) (see also Gogolides, 1994). The ion-ion recombination rate and the detachment frequency (assumed to be due to collisions of CF<sub>4</sub><sup>-</sup> with CF<sub>x</sub> which is present at 1 part in 10<sup>3</sup>) are taken from Gogolides (1994).

SiH<sub>4</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections of Kurachi and Nakamura ((1989). The positive and negative ion mobilities taken from Chatham and Gallagher (1985), and the ion-ion recombination is estimated to be  $5 \times 10^7 \text{ cm}^3 \text{ s}^{-1}$ .

CH<sub>4</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections of Davies et al (1989). The positive and negative ion mobilities and the detachment frequency are also taken from Davies et al (1989).

SF<sub>6</sub>:

The electron mobility, mean energy, ionization and attachment coefficients were calculated using the cross sections of Phelps and Van Brunt (1988). The positive ion mobility is taken from Brand and Jungblunt (1983) (see also Gogolides and Sawin, 1992), and the negative ion mobility is set equal to the positive ion mobility. The ion-ion recombination is taken from Church and Smith (1977) (see also Gogolides and Sawin, 1992).

He:

The electron mobility, mean energy, ionization coefficient were using the same cross sections as in Boeuf (1987). The positive ion mobility as a function of E/p is taken from Ellis et al (1976) .

Ne:

The electron mobility, mean energy, ionization coefficient were calculated the cross sections discussed by Meunier et al (1995). The positive ion mobility as a function of E/p is taken from Ellis et al (1976).

Ar:

The electron mobility, mean energy, ionization coefficient were calculated the cross sections discussed in Fiala et al (1994). The positive ion mobility as a function of E/p is taken from Ellis et al (1976).

Kr:

The electron mobility, mean energy, ionization coefficient were calculated using the cross sections of Date et al (1989). The positive ion mobility as a function of E/p is taken from Ellis et al (1976).

Xe:

The electron mobility, mean energy, ionization coefficient were calculated using the cross sections discussed by Meunier et al (1995). The positive ion mobility as a function of E/p is taken from Ellis et al (1976).

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