

NCPL - On-line tool for evaluation of parameters of non-equilibrium near-cathode plasma layer in high-pressure arc plasmas

<http://fisica.uma.pt/public/NCPL>

Instruction for use

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Evaluation of parameters of non-equilibrium layers at thermionic cathodes of arc discharges as functions of the local cathode surface temperature T_w and the near-cathode voltage drop U is an indispensable element of self-consistent modelling of high-pressure arc discharges [1]. The code NCPL performs such evaluation with the use of the model [2-4]; a summary of equations of the model is given in [5]. In particular, the code computes:

- The density of energy flux from the plasma to the cathode surface, $q(T_w, U)$;
- The density of electric current from the plasma to the cathode surface, $j(T_w, U)$;
- The electron temperature in the near-cathode layer, $T_e(T_w, U)$;
- The pressure exerted over the cathode surface by the near-cathode plasma, $p_{pl}(T_w, U)$, evaluated as sum of the pressure in the bulk plasma and the electrostatic force, applied by the electric field to the near-cathode layer per unit area [6].

The database of plasma-producing gases includes, but is not limited to, He, Ne, Na, Ar, Cu, Kr, Xe, Cs, Hg, air, mixtures Na-Hg and Cs-Hg, plasmas of mercury or xenon with addition of metal halides.

I. Specifying input parameters

Plasma-producing gas

If you wish to work with a pure monoatomic plasma-producing gas, just enter in this field the chemical symbol, e.g., He. The first character must be non-blanc. Please observe the difference between upper and lower-case letters. The code will use atomic parameters and other data needed for calculation of the near-cathode plasma layer (the rate constants of direct and stepwise ionization of atoms by electron impact and cross-section for momentum transfer in elastic collisions ion-atom) for the gas being considered, taken from the internal database. This version of the database includes, but is not limited to, He, Ne, Na, Ar, Cu, Kr, Xe, Cs, and Hg; if the gas you wish to work with is not in the database, the code will issue an error message and terminate. This version of the database allows also working with the following mixtures: air (entry: ai),

mixture Na-Hg (entry: NH), mixture Cs-Hg (entry: CH), plasmas of mercury with addition of metal halides (entry: MH; the percentage of additives is assumed to be small), plasmas of xenon with addition of metal halides (entry: XH; the percentage of additives is assumed to be small).

Plasma pressure

Enter pressure in the bulk plasma (in bars). For instance, 1 is a suitable approximation for most atmospheric-pressure arcs.

Cathode material

Enter in this field the chemical symbol of metal which the cathode is made of, e.g., W. The first character must be non-blanc; for example, 'W' is permitted while ' W' will cause an error message and the code will terminate. Observe the difference between upper and lower-case letters. The code will use the temperature-dependent thermal conductivity, the temperature-dependent hemispherical total emissivity, and thermionic emission properties for the specified cathode material, taken from the internal database. This version of the database includes, but is not limited to, W, Mo, Hf, Fe, Nb, and Zr; if you specified a metal which is not in the database, the code will issue an error message and terminate.

Radiation

Enter .t. (true) if you wish to take into account the cooling of the surface of the cathode by radiation. In this case, the (net) energy flux from the plasma to the cathode surface, $q(T_w, U)$, will be evaluated as the difference between the energy flux transported to the surface by the ions and the electrons and the radiative cooling of the cathode surface, evaluated in terms of T_w and the temperature-dependent hemispherical total emissivity of the cathode material taken from the internal database. Enter .f. (false) if you wish to neglect the radiative cooling. In this case, only the energy flux transported by the ions and the electrons will be taken into account.

Emission parameters will be taken from the internal database

The code evaluates the density of electron emission current from the cathode by means of the Richardson-Schottky formula or the Murphy-Good theory. (The Murphy-Good theory is realized by means of the method [7], which employs Padé approximants and is computationally efficient in the full range of conditions of validity of the theory, from field to thermo-field to thermionic emission regimes.) Properties of the emitting material are characterized in the framework of the standard Murphy-Good theory by just one parameter, the work function. On the other hand, two parameters appear in the Richardson-Schottky formula: in addition to the work function, the factor in front of the exponent is represented as $A_{em} = \lambda_R A_0$, where A_0 is a universal constant given by $A_0 = 4 \pi m_e k^2 e / h^3 \approx 1.2017 \times 10^6 \text{ A}/(\text{m K})^2$ and λ_R is a material-specific correction factor, which is typically of order 0.5. The code introduces the same correction factor λ_R also into the Murphy-Good theory, i.e., the emission current density, given by the standard Murphy-Good theory, is multiplied by λ_R . (This is done in order to ensure that the results given by the Murphy-Good theory in the thermionic emission limit be consistent with those given by the Richardson-Schottky formula.)

Thus, we need to specify two electron emission parameters: the work function and the pre-exponential factor A_{em} . If you leave the default value Yes in the field Emission

parameters will be taken from the internal database, the code will employ (constant) values of these parameters for the specified cathode material, taken from the

internal database. Choose the value No if you want to specify these values by yourself. (This option is particularly useful while working with doped materials, e.g., thoriated tungsten.) A further option, which is available in the case where the cathode material is tungsten and the plasma-producing gas is one of the mixtures Na-Hg or Cs-Hg, is to make the code evaluate the work function taking into account its variation owing to the formation of a monolayer of alkali metal atoms on the surface [3].

Work function

(This field is present on the screen if you entered No in the field Emission parameters will be taken from the internal database.) Enter here the work function you are going to use (in eV).

Pre-exponential factor in the Richardson-Schottky formula

(This field is present on the screen if you entered No in the field Emission parameters will be taken from the internal database.) Enter here the pre-exponential factor in the Richardson-Schottky formula you are going to use (in $A / m^2 K^2$).

Variability of the work function

(This field is present on the screen if you entered No in the field Emission parameters will be taken from the internal database.) Leave the default value .f. in this field if you want the code to employ the (constant) values of the emission parameters specified in the fields Work function and Pre-exponential factor in the Richardson-Schottky formula. Choose the value .t. if you want the code to evaluate the (variable) work function of tungsten covered with sodium (plasma-producing gas = NH) or cesium (plasma-producing gas = CH) atoms [3]. (Values that appear in the fields Work function and Pre-exponential factor in the Richardson-Schottky formula have no effect in this case.) Attention: if this field reads .t., then cathode should be W and gas either NH or CH, otherwise the code will issue an error message and terminate. Note that the modelling with account of variations of the work function requires special care, especially in the case of CH plasma.

Field enhancement factor

Enter 0 in this field if you want the code to employ the Richardson-Schottky formula while evaluating the electron emission. If the field enhancement factor (FEF) is positive, then the Murphy-Good formalism is used with the electric field being equal to the field given by the cathode sheath equations multiplied by the FEF value.

Effective secondary electron emission coefficient

The secondary electron emission is introduced in terms of the so-called effective secondary emission coefficient, which is assumed to characterize all mechanisms of secondary electron emission (due to ion, photon, and excited species bombardment; e.g., section 4.7.2 of Raizer 1991).

Content of sodium, Content of thallium, Content of dysprosium,
Content of scandium, Content of cesium, Content of zinc, Content
of indium, Content of thorium, Content of iodine

These fields are relevant if your plasma-producing gas is CH, or NH, or MH, or XH; see tutorial of the UMa online tool for modelling of arc-cathode interaction, http://www.arc_cathode.uma.pt/tool/tutorial.pdf, for details.

If you need to perform simulations for a cathode material that is not included in this version of the database:

- Specify appropriate values of the emission parameters and set `radiative_cooling = .f.`
- Run the code.
- Evaluate yourself the radiative cooling for your cathode material and subtract it from the function q values given by the code.

II. Specifying output format

The evaluation is performed in the rectangular domain $T_{wlo} \leq T_w \leq T_{whi}$, $U_{lo} \leq U \leq U_{hi}$. There are $(nT_w + 1)$ values of T_w that are equally spaced over the interval $[T_{wlo}, T_{whi}]$ and $(nU + 1)$ values of U that are equally spaced over the interval $[U_{lo}, U_{hi}]$. Thus, you need to specify T_{wlo} , T_{whi} , U_{lo} , U_{hi} , and the numbers of steps nT_w and nU .

If $nT_w=0$, the code will run only for $T_w=T_{wlo}$; T_{whi} is irrelevant in this case.

If $nU=0$, the code will run only for $U=U_{lo}$; U_{hi} is irrelevant in this case.

T_{whi} should be normally chosen sufficiently high for the function $q(T_w, U)$ to change sign from plus to minus. (The value of T_w at which this happens gives an estimate of the cathode surface temperature inside spots.) On the other hand, the code in some cases may stop working at T_w too high. The value $T_{whi}=7kK$ seems to be a safe bet in all the cases. However, you may wish to choose a smaller value in order to reduce the size of the tables.

Sometimes, the code may terminate unexpectedly with a message like this:

```
From CVC_U: unable to initiate bisection for
```

```
Tw = 5200K,      U = 8900.0000V
```

```
Check the file "manual_NCPL.pdf". The code terminated.
```

Usually this happens if U is very low or very high. In the first case, this happens in the range of lower T_w ; e.g., for Ar_1bar/W and $U = 4.9V$ this happens in the range $T_w \leq 4100K$. In the case where U is very high, this happens in the range of higher T_w ; e.g., for Ar_1bar/W and $U = 8.9kV$ this happens in the range $T_w \geq 5200K$.

Normally, values of U that low or high are irrelevant for arc cathodes. If, for some reason, you do need to perform computations for these conditions, a fine-tuning of the engine (subroutine CVC_U, created by Mikhail Benilov) will be required.

T_w_0

Normally, T_w_0 may be set equal to any value below T_{wlo} , then the exact value of T_w_0 has no effect.

Higher values of T_w_0 may be required in cases of complex plasma composition (actually, this option was introduced for $gas = MH$ or XH), where the code does not converge for low T_{wlo} and zero effective secondary electron emission coefficient. In such cases, you may try setting T_w_0 equal to a

value above T_{w0} , then the code will neglect the presence of ionization near the cathode in the range $T_{w0} \leq T_w \leq T_{w_0}$. (The thermionic emission current is evaluated by means of the Richardson formula and radiation cooling of the cathode surface is taken into account.) An alternative is to introduce 0.D0 into in this field, then the default value of T_{w_0} is used, which is 1000K for $gas = MH$ or XH and 500K for all other cases.

Detailed printout

Check `.t.` (true) if you wish a detailed printout to be produced. Check `.f.` (false) if you wish to reduce the size of data to be transferred.

III. Running the code

Press the button `Start Calculations`. The window in the right-hand part of the screen will show the progress of the code. When the code has finished, it will offer you to save the file `results.zip`, which contains the output. The output includes, in particular, the files `q.dat` (the density of energy flux from the plasma to the cathode surface, $q(T_w, U)$); `j.dat` (the density of electric current from the plasma to the cathode surface, $j(T_w, U)$); `Te.dat` (the electron temperature in the near-cathode layer, $T_e(T_w, U)$); and `pl_pres.dat` (the pressure exerted over the cathode surface by the near-cathode plasma, $p_{pl}(T_w, U)$, as defined in [6]).

The files have the following structure (value = the corresponding value of q, j, T_e , or p_{pl}):

<code>Twlo</code>	<code>Ulo</code>	value
<code>Twlo+DelTw</code>	<code>Ulo</code>	value
<code>Twlo+2*DelTw</code>	<code>Ulo</code>	value
<code>...</code>		
<code>...</code>		
<code>Twhi</code>	<code>Ulo</code>	value
<code>Twlo</code>	<code>Ulo+DelU</code>	value
<code>...</code>		
<code>...</code>		
<code>Twhi</code>	<code>Ulo+DelU</code>	value
<code>Twlo</code>	<code>Ulo+2*DelU</code>	value
<code>...</code>		
<code>...</code>		
<code>Twhi</code>	<code>Uhi</code>	value

All values are in SI, `DelTw` and `DelU` are steps over T_w and U , respectively.

The output includes also a file with a name like `Ar_001bar_parameters.dat`, containing parameters for which the calculation has been performed. If you have checked `.t.` in the field `Detailed printout`, then the output includes also a file with a name like `Ar_001bar_detailed.dat`, containing detailed information.

No plasma is present near the cathode at T_w low enough. In this case, the code evaluates the density of electric current from the plasma to the cathode in the file `j.dat` assuming that it is purely electron thermionic emission current, so the Richardson formula is used. The energy flux density in the file

q.dat is evaluated as the thermionic cooling to which the radiation cooling is added (if radiation=.t.) No information is written in the files Te.dat and Ar_001bar_detailed.dat.

It may be that the data files contained in results.zip are incomplete or even empty, i.e., contain only headers. This means that the code has terminated unexpectedly (for example, this happens if the specified gas is not in the database) and the error message can be found in the window in the right-hand part of the screen.

IV. If the code runs on your computer

The above refers to the case where you run the code via Internet on a server of Universidade da Madeira. If you have received from us a Windows version of the code and run it on your computer, the following changes should be introduced into the above.

The standard distribution of the code includes, apart from this file (manual_NCPL.pdf), four files: ncpl.exe, input.dat, parameters_of_run_ncpl.dat, cmd.bat. Copy these four files into a working folder.

The input parameters are specified by editing the file input.dat (any ASCII editor can be used). The file is self-explaining. Note that the value 0.D0 in the 9th and/or 10th lines (user-specified values of the work function and the pre-exponential factor in the Richardson-Schottky formula) instructs the code to use values of the work function and the pre-exponential factor for the given cathode material from the internal database. Alternatively, you can specify emission parameters yourself. Values in the fields cathode radius, cathode height, temperature of the cathode base, and lateral surface is insulating or not are irrelevant and need not be changed.

Values Twlo, Twhi, Ulo, Uhi, the numbers of steps over T_w and U , and Detailed printout are specified by editing the file parameters_of_run_ncpl.dat. The file is self-explaining.

When you are done with the editing, click the file cmd.bat. A DOS window will open. Type in this window ncpl and press Enter. You will see in this window the progress of the code. After the code has finished, the output is written into the files q.dat, j.dat, Te.dat, pl_pres.dat, Ar_001bar_parameters.dat, and Ar_001bar_detailed.dat, created in the current folder.

References

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