

# NCPL – A tool for evaluation of parameters of non-equilibrium near-cathode plasma layer in high-pressure arc plasmas

<https://fisica.uma.pt/public-domain/simulation-tools/ncpl/>

## Manual

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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 high-current arc discharges [1]. The code NCPL performs such evaluation with the use of the model summarized in Appendix A of [2] and updated as discussed in [3]. The updated model describes glow-like discharges on cold cathodes and thermionic arc discharges on hot cathodes, which makes possible multidimensional simulations not only of arc discharges on thermionic cathodes, but also of the ignition of high-current arcs on cold refractory cathodes.

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 [4].

These functions may be used to simulate the cathodic part of the arc and to produce boundary conditions for the 2T or LTE MHD equations describing the arc bulk.

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.

The users may run [the code online](#) on a server of Departamento de Física of Universidade da Madeira or, alternatively, download a [Windows version of the code](#) and run it on user's PC.

### Conditions of use

The code is free for non-commercial personal use only. Simulation results must not be transferred to third parties, however they may be used for producing scientific publications, provided that the references are made to the papers [2] and [3] and to this site (<https://fisica.uma.pt/public-domain/simulation-tools/ncpl/>).

## Disclaimer

The code is made available "AS IS" without warranty of any kind. The entire risk as to the results and the performance of the code is assumed by the user, and in no event will the authors be liable for any consequential, incidental or direct damages suffered in the course of using the code.

## 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.

If you need to perform simulations for a cathode material that is not included in this version of the database, then set `radiative cooling = .f.`, specify appropriate values of the electron emission parameters (see below), run the code, evaluate yourself the radiative cooling for your cathode material and subtract it from the function  $q$  values given by the code.

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 [5], 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  $\lambda_R$  is a material-specific correction factor, which is typically of order 0.5. The code accounts for the same correction factor  $\lambda_R$  also into the Murphy-Good theory, i.e., the emission current density, given by the standard Murphy-Good theory, is multiplied by  $\lambda_R$ . (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 possibility, 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 [6].

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  $\text{A} / \text{m}^2 \text{K}^2$ ).

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 [6]. (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 (This option is unavailable in the online version of the code)  
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 (This option is unavailable in the online version of the code)  
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

If your plasma-producing gas is NH, or MH, or XH, enter in this field the mole fraction of the element of sodium in the mixture. This field has no effect if your plasma-producing gas is neither NH nor MH nor XH.

Content of thallium

If your plasma-producing gas is MH or XH, enter in this field the mole fraction of the element of thallium in the mixture. This field has no effect if your plasma-producing gas is neither MH nor XH.

Content of dysprosium

If your plasma-producing gas is MH or XH, enter in this field the mole fraction of the element of dysprosium in the mixture. This field has no effect if your plasma-producing gas is neither MH nor XH.

Content of scandium

If your plasma-producing gas is MH or XH, enter in this field the mole fraction of the element of scandium in the mixture. This field has no effect if your plasma-producing gas is neither MH nor XH.

Content of cesium

If your plasma-producing gas is CH, or MH, or XH, enter in this field the mole fraction of the element of cesium in the mixture. This field has no effect if your plasma-producing gas is neither CH nor MH nor XH.

Content of zinc

If your plasma-producing gas is XH, enter in this field the mole fraction of the element of zinc in the mixture. This field has no effect if your plasma-producing gas is not XH.

Content of indium

If your plasma-producing gas is XH, enter in this field the mole fraction of the element of indium in the mixture. This field has no effect if your plasma-producing gas is not XH.

Content of thorium

If your plasma-producing gas is XH, enter in this field the mole fraction of the element of thorium in the mixture. This field has no effect if your plasma-producing gas is not XH.

Content of iodine

If your plasma-producing gas is XH, enter in this field the mole fraction of the element of iodine in the mixture. This field has no effect if your plasma-producing gas is not XH.

In the case of metal halide plasmas (MH) the code evaluates mole fraction of the element of iodine assuming that the metal halides are added to mercury in the form of molecules NaI, TlI, DyI<sub>3</sub>, ScI<sub>3</sub>, CsI. In other words, mole fraction of the element iodine is evaluated in terms of mole fractions of the elements Na, Tl, Dy, Sc, and Cs as  $ZI = ZNa + ZTl + 3(ZDy + ZSc) + ZCs$ . It is assumed that the only element of metal halide plasmas besides Na, Tl, Dy, Sc, Cs, and I is Hg, i.e., the code assumes  $ZHg = 1 - (ZNa + ZTl + ZDy + ZSc + ZCs + ZI)$ .

In the case of plasmas of xenon with addition of metal halides (XH), it is assumed that the only element of the plasmas besides Na, Tl, Dy, Sc, Cs, Zn, In, ZTh, and I is Xe, i.e., the code assumes  $ZXe = 1 - (ZNa + ZTl + ZDy + ZSc + ZCs + ZZn + ZIn + ZTh + ZI)$ .

## II. Specifying output format

$T_{wlo}$ ,  $T_{whi}$ ,  $n_{Tw}$ ,  $U_{lo}$ ,  $U_{hi}$ ,  $n_U$

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  $(n_{Tw} + 1)$  values of  $T_w$  that are equally spaced over the interval  $[T_{wlo}, T_{whi}]$  and  $(n_U + 1)$  values of  $U$  that are equally spaced over the interval  $[U_{lo}, U_{hi}]$ .

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

If  $n_U=0$ , 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.

Sequence (This option is unavailable in the online version of the code)

The evaluation is performed for the following pairs of  $(T_w, U)$  values:

$T_{wlo}, U_{lo}$	$T_{wlo} + \Delta T_w, U_{lo}$	...	$T_{whi}, U_{lo}$
$T_{wlo}, U_{lo} + \Delta U$	$T_{wlo} + \Delta T_w, U_{lo} + \Delta U$	...	$T_{whi}, U_{lo} + \Delta U$
...	...	...	...
$T_{wlo}, U_{hi}$	$T_{wlo} + \Delta T_w, U_{hi}$	...	$T_{whi}, U_{hi}$

[Here  $\Delta T_w = (T_{whi} - T_{wlo})/n$  and  $\Delta U = (U_{hi} - U_{lo})/n$  are steps over  $T_w$  and  $U$ , respectively.] Set Sequence equal to 1 if you want the printout to be arranged in the line sequence (i.e., first the results for each pair  $(T_w, U)$  in the first line, then in the second line etc). Set Sequence equal to 2 if you want the printout to be arranged in the column sequence (i.e., first the results for each pair in the first column, then in the second column etc).

$T_{w\_0}$  (This option is unavailable in the online version of the code)

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  $T_{wlo}$ , then the code will neglect the presence of ionization near the cathode in the range  $T_{wlo} \leq T_w \leq T_{w\_0}$ . (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 online

Open the Internet page <https://fisica.uma.pt/ncpl/> and fill all fields as appropriate. 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 [4]).

The files have the following structure (value = the corresponding value of  $q, j, T_e$ , or  $p_{pl}$ ; this example refers to `Sequence=1`):

Twlo	Ulo	value
Twlo+DelTw	Ulo	value
Twlo+2*DelTw	Ulo	value
...		
...		
Twhi	Ulo	value
Twlo	Ulo+DelU	value
...		
...		
Twhi	Ulo+DelU	value
Twlo	Ulo+2*DelU	value
...		
...		
Twhi	Uhi	value

All values are in SI.

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. Running the code on your PC

The previous section refers to the case where you run the code online on a server of Departamento de Física of Universidade da Madeira. If you have downloaded a [Windows version of the code](#) and run it on your PC, 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.DO` in the 9<sup>th</sup> and/or 10<sup>th</sup> 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

- [1] M. S. Benilov, [Modeling the physics of interaction of high-pressure arcs with their electrodes: advances and challenges](#), J. Phys. D: Appl. Phys. **53**, No. 1, p. 013002 (2020).
- [2] M. S. Benilov, M. D. Cunha, and G. V. Naidis, [Modelling interaction of multispecies plasmas with thermionic cathodes](#), Plasma Sources Sci. Technol. **14**, No. 3, pp. 517-524 (2005).
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- [4] M. D. Cunha, H. T. C. Kaufmann, D. F. N. Santos, and M. S. Benilov, [\*Simulating changes in shape of thermionic cathodes during operation of high-pressure arc discharges\*](#), J. Phys. D: Appl. Phys. **52**, No. 50, p. 504004 (2019).
- [5] M. S. Benilov and L. G. Benilova, [\*Field to thermo-field to thermionic electron emission: A practical guide to evaluation and electron emission from arc cathodes\*](#), J. Appl. Phys. **114**, No. 6, pp. 063307-1-7 (2013).
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