Code for derivation of parameters of z-pinch plasma of any chemical composition with any distribution of free electrons

The code follows thermodynamic scenario that **user expects** for z-pinch plasma in terms of two radial zones. While advancing along this scenario, the code computes spectral power radiated in side-on direction, signals of PCDs (*of prescribed spectral response*), spectrograms taken at requested times. Comparing computed data to that in experiment, **user may improve his scenario** until satisfied with the comparison, thus finding parameters of plasma.

I. Advantages of the code

1. It accounts the **effects caused by presence of few chemical elements in plasma,** in particular, the code is rigorous in simulation of merging spectral lines of all species. This advantage is important for deriving parameters of plasma from comparison of computed spectrograms to those in experiments.
2. **Users can prescribe any distribution of free electrons over energy.** Due to this option, users may analyze consequences of generation of electron beam in plasma as well as consequences of other deviations from Maxwellian distribution.
3. We did not assume any type of equilibrium in plasma; therefore, the computations are **correct for plasmas with arbitrarily quick changes in parameters and in the distribution of electrons.** Moreover, the code may be used for computation of time required for equilibration of ion level populations, thus ionization composition and radiation as well.
4. The code may be converted in **post-processor of hydrodynamic simulations**. This post-processor will compute spectral power radiated by z-pinch plasma, signals of PCDs, sequence of spectrograms (e.g. frames of TREX) at requested times.

II. The model and the code

The code is written for derivation of parameters of **z-pinch plasma**. In the model, cylindrical on-axis **core** of radius $R_1(t)$ is surrounded by **halo** of inner radius $R_1(t)$, outer radius $R_2(t)$. Both zones are of length L(t). Within each zone plasma is uniform. Zones affect each other by **radiation**. L(t), $R_1(t)$, $R_2(t)$, thermodynamic parameters of plasma follow scenario **to be prescribed** in file *Params2.inp*. Based on comparison of computed to experimental data, **user can improve** his scenario and repeat computations until satisfied by comparison; it gives him an estimate of dimentions and parameters of plasma.

One of advantages of present code is **rigorous account of chemical composition**. This is important for plasmas of complex composition, e.g. plasmas of alloys or gas mixes. **User can choose** chemical composition following explanation in Section IV.

Diagnostics at hν > 1 keV restricts the electron temperature to

$$T_{e,b}(t) > 100 \text{ eV}, \qquad \text{(II. 1)}$$

subscript $b = 1$ denotes core, $b = 2$ denotes halo. Each of these two zones is characterized with time-dependent parameters as follows:

(i) **ion number densities** $n_{a,b}(t)$ in units [cm^{-3}]; $a = 1, 2, 3, 4$ is serial number of chemical element in database of the code.

(ii) **distribution f_b of free electrons over their energy ε_e.**

No restrictions on $f_b(\varepsilon_e, t)$ except $\int_0^\infty f_b(\varepsilon_e, t)\, d\varepsilon_e = 1$. Units of ε_e and f_b are [eV] and [eV^{-1}], respectively. **User may prescribe** any $f_b(\varepsilon_e, t)$ in "*function EED*" in file "*Code_4.for*".
The possibility of choosing $f_b(\varepsilon_e, t)$ is substantial advantage of present code. In particular, this option enables simulations and analysis of spectra radiated by plasma with electron beam(s).

To compute transition rates for any $f_b(\varepsilon_e, t)$, **each transition is given by its cross-section** (not by commonly used maxwellian rate). The cross-sections are computed using Flexible Atomic Code **[1]**. In demo version of the code $f_b(\varepsilon_e, t)$ consists of maxwellian and beam parts:

$$f_b(\varepsilon_e, t) = (1 - \xi_b)\, f_{\text{Maxw}}(\varepsilon_e, T_{e,b}) + \xi_b\, f_{\text{beam}}(\varepsilon_e, \varepsilon_{e,c,b}, \varepsilon_{e,w,b}) \qquad \text{(II. 2)}$$

where $f_{\text{Maxw}}(\varepsilon_e, T_{e,b})$ is Maxwell distribution for $T_{e,b}(t)$; parameter $\xi_b(t)$ is the beam part of local number density of free electrons; $f_{\text{beam}}(\varepsilon_e, \ldots)$ is the shape of electron beam. In demo version of the code this shape is rectangular; $\varepsilon_{e,c,b}(t)$, $\varepsilon_{e,w,b}(t)$ are central energy and width of e-beam. Functions f_{Maxw}, f_{beam} are each normalized to the under-shape area = 1. Cross-section of elastic e-e collisions $\sim \varepsilon_e^{-2}$ **[2]**, therefore interaction between high-energy e-beam [*that with* $(\varepsilon_{e,c,b} - \varepsilon_{e,w,b}/2) \gg T_{e,b}$] and maxwellian electrons is negligible, therefore two terms of (II.2) don't mix.

(iii) **mean absolute velocity of 3D motion of ions**, $u_{3D,b}$. This parameter characterizes distribution of ion velocity in two simultaneous motions that are local thermal motion of individual ions and their collective hydro motion in zone b.

- **Time dependence** of R_b, $n_{a,b}$, $T_{e,b}$, $u_{3D,b}$, ξ_b, $\varepsilon_{e,c,b}$, $\varepsilon_{e,w,b}$ **must be prescribed** in file "*Params2.inp*".
- For each chemical element, the database of the code **must** provide info on nuclei, H-like, He-like, Li-like ions and **can** include info on ionization stages below Li-like; all ionization stages must follow in one sequence (no missing stages) down to a stage which has the ionization energy of its ground state $I_{a,q} < 1$ keV; here q

denotes the ion charge. We omit lower q because at $T_{e,b} > 100$ eV their population is negligible. More info on database of the code and instruction for replacement are given in Section IV.

- **Number density of free electrons in zone *b*** is given by the equation of plasma neutrality

$$n_{e,b} = \sum_a Z_{a,b}\, n_{a,b} \qquad \text{(II. 3)}$$

where $Z_{a,b}$ is the mean charge of ions of chemical element a in zone b; computed $Z_{a,b}$ depend on database of energy levels, method of computation of inelastic cross-sections, model of the lowering of continuum in plasma.

- **Number density of ions in zone *b***

$$n_b = \sum_a n_{a,b}$$

Let $n_{a,b,l}$ denote the number density of ions of chemical element a on the energy level l in zone b. Sum over the levels

$$\sum_l n_{a,b,l} = n_{a,b}. \qquad \text{(II. 4)}$$

Functions $n_{a,b,l}\ (t)$ are computed by integration of the system of rate equations of the level-population kinetics **[3-5]**

$$dn_{a,b,l}/dt = \sum_{l' \neq l} W_{l',l}\, n_{a,b,l'} - n_{a,b,l} \sum_{l' \neq l} W_{l,l'} \qquad \text{(II. 5)}$$

On each time step, the code integrates system (II.5) for each a,b separately but accounts a transfer of radiation between zones, *see below*. $W_{l',l}$ is the probability of $l' \rightarrow l$ transition due to all possible for this pair. The code chooses them from ionization, three-body recombination, excitation, deexcitation (*all caused by impacts of free electrons*), spontaneous and photoinduced radiative transitions (spectral lines and radiative recombination), photoionization, photoexcitation, photodeexcitation, autoionization, dielectronic recombination.

Computation of probabilities of photostimulated transitions in zone b requires **space- direction- average spectral intensity of radiation in this zone, $J_{\nu,b}(t)$**. We approximated $J_{\nu,b}$ by a mean of solutions of the equation of radiation transfer along six lines of sight (**LOS**s) directed towards "representative" point (RP) of zone b. For both zones RP is chosen at z = L/4. Radial coordinate of RP is chosen at $r_c = R_1/2$ for core, $r_h = (R_1 + R_2)/2$ for halo. Six LOSs are chosen along three cartezian axes: x along r, axis z along z-pinch axis, axis y perpendicular to x, z. Part of the LOSs cross both zones therefore **$J_{\nu,b}(t)$ depends on scenario chosen for both zones**. Function $J_{\nu,b}$ and contribution of each LOS are shown in file "*EffSpIns.dat*" in units [W/eV/sr/cm^2].

Due to differential eqs. (II.5) present code has advantage over widely used collisional-radiative equilibrium (CRE) codes because, by definition, they assume $dn_{a,b,l}/dt = 0$, thus simplify system (II.5) to algebraic equations, that means immediate relaxation of each $n_{a,b,l}$ to instant parameters of plasma. Computations show that this assumption is often wrong; namely, level populations depend on entire scenario for the period $t_0 \rightarrow t$. Present code may be used for determination of time, t_{CRE}, needed for relaxation of $n_{a,b,l}(t)$ to their CRE distribution at parameters of interest, *see the last paragraph in Section V*.

The code integrates system (II.5) by the 4th order Runge-Kutta method using *D02EAF* subroutine of NAG library. At t_0 the code loads all ions of a on one energy level ***to be chosen*** *in file "Params1.inp"*. In the demo package of files, this level is the ground state of He-like ions for each a,b; other levels are given initial population $n_{a,b,l} = 0$. With time, the radiation and collisions distribute $n_{a,b,l}(t)$ over all energy levels according to probabilities

of transitions, thermodynamic scenario and $J_{\nu,b}(t)$ which, in turn, depends on $n_{a,b,l}(t)$. Thus obtained $n_{a,b,l}(t)$ are used in solution of the equation of radiation transfer along side-on LOSs, *see next Section*.

Lowering of the ionization energy of ions a^{q+} is denoted $\Delta I_{a,q,b}$ and taken in the Ion Sphere approach. In Appendix we show that in neutral plasma

$$\Delta I_{a,q,b} = 2(q+1) I_H \zeta_0 / \zeta_{q,b}, \qquad \text{(II. 6)}$$

where $I_H = 13.606$ eV is the Rydberg energy, $\zeta_0 = 0.52918 \times 10^{-8}$ cm is Bohr radius, $\zeta_{q,b} = [3q/(4\pi n_{e,b})]^{1/3}$ is radius of ion sphere of a^{q+}.

III. Radiation power towards side-on detectors, computation of spectrograms and signals of PCDs.

Plasma emissivity $\varepsilon_{\nu,b}$ is due to bound-bound, free-bound, free-free transitions of electrons. Absorption coefficient corrected for stimulated emission $\kappa'_{\nu,b}$ is due to bound-bound, bound-free, free-free transitions. In the code, the units of $\varepsilon_{\nu,b}$ are [W/eV/cm^3/sr], the units of $\kappa'_{\nu,b}$ are [cm^{-1}]. In the bound-bound part of $\varepsilon_{\nu,b}$, $\kappa'_{\nu,b}$ each spectral line is given **voigt shape** with **gaussian part of the width** defined by Doppler broadening (thus by $u_{3D,b}$), **lorentzian part of the width** defined by bigger of two: Stark effect or the uncertainty principle. In the computations of Stark width we follow Refs. **[6,7]**. For the uncertainty principle, life time of excited states is taken in Baranger' approach **[4]**. Gaussian and lorentzian parts of width of each line are shown in files "*CoreLineInfo.dat*", "*HaloLineInfo.dat*", for details see Section VI.

Spectral power of plasma radiation towards detector [W/eV/sr]

$$P_\nu(t) = L(t) \int_{-R2}^{R2} I_\nu(y,t)\, dy \ . \qquad \text{(III.1)}$$

where y is the height of a LOS above z-pinch axis, $I_\nu(y,t)$ is spectral intensity of plasma radiation on the exit of this LOS, i.e. solution of the equation of radiation transfer along a LOS through plasma column towards detector.

Spectral power (III.1) is used for computation of signals of three PCDs, eigth spectrograms (e.g. frames of TREX). Duration of a frame, spectral interval of spectrograms, instrumental broadening **to be chosen** in file "*Params1.inp"*; timing of the frames **to be prescribed** in file "*Params2.inp"*. Computed spectrograms will be printed in file "*Frames.dat*". For comparison to experimental data, computed spectrograms **should be multiplied** by spectral response of the instrument. In demo version of the code we computed PCD signals using spectral response of diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (those used in Z shot 1520), see files

"*Respo5milKapPCD.inp*",
"*Respo10milKapPCD.inp*",
"*Respo40milKapPCD.inp*".

For other PCDs these files should be replaced by response curves of those PCDs. Computed PCD signals will be printed in file "*PCDs.dat*" in Watts. More details are given in Section VI.

IV. Source file and input files

Source file of present code is *"Code4.for"* written in the **Microsoft Fortran for Power Station**. "*Code4.for*" and module *"mo1code4.for"* should be compiled using **Microsoft Developer Studio**.

Atomic database of demo version of the code corresponds to chemical composition of stainless steel **[8]** and consists of files

"QSsFe.inp", "QSsCr.inp", "QSsNi.inp", "QSsMn.inp",
"InzFe.inp", "InzCr.inp", "InzNi.inp", "InzMn.inp",
"AIwFe.inp", "AIwCr.inp", "AIwNi.inp", "AIwMn.inp",
"ExcFe.inp", "ExcCr.inp", "ExcNi.inp", "ExcMn.inp".

For plasma of another composition, these files should be replaced by similar info **printed in format of present files**, *for details, see next four paragraphs.* For each chemical element, the database **must** include info on nuclei, H-like ions, He-like, Li-like ions and **can** include ions of spectroscopic symbols (SpSs) below Li-like; all SpSs must follow in one sequence (no missing SpSs). **Changes in the database** require changes in parameters nXE, FSS, HSS, Nnu, NST, NSTm, HSSm, nFAI introduced and explained in module "*mo1code4.for*".

In demo version of the code, files *"QSsFe.inp", "QSsCr.inp", "QSsNi.inp", "QSsMn.inp"* give info on ions in the highest five SpSs that are Be-like to nucleus. Lines 3-6 give the number of non-autoionizing Els in SpS, the number of autoionizing (AI) Els in SpS, non-lowered ionization energies of the ground states of SpS (*computed using FAC* **[1]**. Lines from 9 till the end of file give info on each energy level (EL):

columns 1,2 give electron configuration of EL,
column 3 gives the degeneracy of EL,
column 4 gives its energy above the ground state,
column 6 gives serial number of EL among ELs of same-charge ions;
in this column AI ELs are placed below nucleus; for convenience of programming, AI ELs are given numbers > 200;
column 7 gives serial number of EL in the full list of ELs of this chemical element.

In demo version of the code, files *"AIwFe.inp", "AIwCr.inp", "AIwNi.inp", "AIwMn.inp"* give autoionization (AI) probabilities of energy levels (ELs) of Fe, Cr, Ni, Mn, respectively. The probabilities are computed using FAC.

Column 1, 2 give spectroscopic symbol (SpS) and serial number of AI EL.
Columns 3,4 give SpS and serial number of final (after AI) EL.
Column "WAI" gives the probability of AI.
Column DE gives the difference [eV] between energies of initial and final ELs prior to the lowering of continuum.

In demo version of the code, files *"ExcFe.inp", "ExcCr.inp", "ExcNi.inp", "ExcMn.in"* give cross-sections of excitation of ELs by electron-impact. The cross-sections are computed with FAC. Column 1 gives SpS of an ion. Column 2 gives serial number of initial (lower) EL in the list of ELs of this SpS. Column 3 gives serial number of final (upper) EL in this list. Column 4 gives the number of formula used for interpolation of cross-section computed with FAC, see *function "SigExc(eeV)"* in the code. Columns 5 - 10 give coefficients for this interpolation formula. Sign "-" in column 11 is a **mark**; it marks a computation with FAC. Absolute value in column 11 is the absorption oscillator strength of this transition.

In demo version of the code, files *"InzFe.inp", "InzCr.inp", "InzNi.inp", "InzMn.inp"* give cross-sections of ionization of ELs by electron impact. The cross-sections are computed with FAC. Column 1 gives SpS of an ion. Column 2 gives serial number of EL to be ionized (*the number in the list of ELs of this SpS*). Columns 3, 4 display similar info on EL obtained due to the ionization. Columns 5 - 8 display coefficients of formula used for interpolation of computed cross-section, see *function "SigInz(eeV)"* in the source file. Column 9 isn't used in present version. Columns 10 – 13 displays coefficients of formula used for interpolation of computed photoionization cross-sections, see *function "SigPhi(hv)"* in the source file. The last column gives the difference between energies [eV] of initial and final ELs prior to the lowering of continuum.

Files

"Respo5milKapPCD.inp",
"Respo10miKapPCD.inp",
"Respo40miKapPCD.inp"

give spectral response of diamond PCDs with kapton filters 5-, 10-, 40-mils thickness (used in Z shot 1520). The 1st column gives the photon energy [eV], the 2nd column gives response of PCD. $0 \leq$ response ≤ 1. **User can replace** these three files with spectral response of his PCDs. In this case, he **must change** integers "np5kap", "np10ka", "np40ka" in module "*mo1code4.for*". These three integers show number of hν points in the input files.

Files "*Params1.inp*", "*Params2.inp*" **must be filled in by user**. These files give parameters of computation, explanations and/or comments on each parameter. File *Params2.inp* prescribes ion number density $n_{a,b}$ only for a = 1; ion number density of other chemical elements (a = 2, 3, 4) is calculated in subroutine "*Scenario"* based on known quantitative composition of plasma. If less than four elements in plasma, e.g. two, than a = 3, 4 must be given negliginle $n_{a,b}$. In demo version of the code we consider plasma of stainless steel, thus prescribe $n_{a,b}$ of iron, i.e. $n_{Fe,b}(t)$. Ion number density of Cr, Ni, Mn is calculated in subroutine "*Scenario"* based on known percents of mass in composition of stainless steel **[8]**. Note: thermodynamic scenario given in file *Params2.inp* does not correspond to any experiment.

File "*Naglib.lib*" is the part of NAG library, namely, (i) subroutine D02EAF which integrates the system of ordinary differential equations by the 4th order Runge-Kutta method, (ii) definite integral D01AH that we use in computations of transition rates.

Module "*mo1code4.for*" (i) gives parameters that define the size of arrays,
some parameters of database and computations,
(ii) explains the meaning of each parameter.

V. Info on display

On each step in time (denoted "*tstep*" in the source file), the code displays initial instant, t_i, of this *tstep*, parameters of each zone at $t = t_i$, namely, serial nunber of zone (b = 1 for core, b = 2 for halo), outer radius of zone [cm], electron temperature [eV], mean absolute velocity of 3D motion of ions [cm/s], electron density [cm^{-3}], mean charge of ions *(in demo version of the code they are ions of Fe, Cr, Ni, Mn*).

Central time of k-th frame is denoted *FrP(k)*, duration of each frame is *FrL,* both given in file *Params2.inp*. If t_i is within k-th frame, i.e.

$$(FrP(k) - FrL/2) \le t_i < (FrP(k) + FrL/2), \qquad \text{(V.1)}$$

k-th spectrogram is computed as spectral energy collected during k-th frame:

$$\mathrm{FrY}_\nu(k) = \sum_{j=1}^{jmax} tstep \cdot \mathrm{P}_\nu(t_i) ; \qquad \text{(V.2)}$$

here j_{max} is the number of time steps during k-th frame, integer j counts these steps. In the code, *tstep* is constant, FrL is equal for all frames, therefore j_{max} is also equal for all frames. Restriction $tstep \le \mathrm{FrL}/10$ (see 3rd line in file *Params2.inp*) results in $j_{max} \ge 10$. The units of $\mathrm{FrY}(k)$ are [J/eV/sr]. In file *Frames.dat* the units are [J/keV/sr]. Z-pinch spectral power [W/eV/sr] radiated towards detector $\mathrm{P}_\nu(t_i)$ is given by expression (III.1).

During each frame, i.e. for t_i that satisfies inequality (V.1), the code displays k, j.

V. The output files

Files *"CoreInfo.dat", "HaloInfo.dat"* display (i) parameters of plasma in corresponding zones as functions of time [ns], namely: outer radius [cm], electron temperature [eV], mean absolute velocity [cm/s] of ions in their thermal+hydro motion in zone, number density of free electrons [cm^{-3}], mean ion charge in plasma "Z_{bar}", mean charge of ions of each chemical element, number density of ions of each chemical element [cm^{-3}]. Both files are convenient for graphic display of above-mentioned parameters in time.

File "*LineList.dat*" is the list of all spectral lines included in the computation. These are lines which fit three requirements: (i) their centers, $h\nu_C$, are within interval $[h\nu_{min}, h\nu_{max}]$, (ii) absorption oscillator strength $f_{lu} > f_{lu}Min$, (iii) Einstein coefficient $A_{ul} > A_{ul}Min$. Parameters $h\nu_{min}$, $h\nu_{max}$, $f_{lu}Min$, $A_{ul}Min$ are given in file *Params1.inp* . In file "*LineList.dat*"

the 1st column displays serial number of chemical element,
the 2nd column displays spectroscopic symbol of the ion,
the 3rd column displays central energy of the line, $h\nu_C$ [eV],
the 4th column displays the wavelength of the line, λ_C [A],
the 5th column displays A_{ul} [s^{-1}],
the 6th column displays serial number of upper level (that in file *QSs….inp*),
columns 7,8 displays electron configuration of this level,
the 9th column displays serial number of lower level (that in file *QSs….inp*),
columns 10,11 display electron configuration of this level,
the 12th column displays f_{lu}.

Files "*CorLineInfo.dat*", "*HalLineInfo.dat*' display info on FWHM [eV] of spectral lines in corresponding zones. Thesee files include only spectral lines which have (i) centers, $h\nu_c$, within interval [$h\nu_{min}$, $h\nu_{max}$], (ii) the absorption oscillator strength $f_{lu} > f_{lu}Min$, (iii) Einstein coefficient $A_{ul} > A_{ul}Min$. Parameters $h\nu_{min}$, $h\nu_{max}$, $f_{lu}Min$, $A_{ul}Min$ are given in file *Params1.inp* .
In *files "...LineInfo.dat"* :

column "hvCeV" displays $h\nu_c$ [keV],
column "XE" displays serial number of chemical element in database (a),
column "SpS" displays spectroscopic symbol of ion
which radiated this line,
column "Lambda" displays the line-center wavelength [A],
three columns "Upper" display serial number and electron configuration
of upper level of this line,
three columns "Lower" display serial number and electron configuration
of lower level of this line,
column "Gauss" displays FWHM of Gaussian distribution caused by u_{3D},
column "Baranger" displays FWHM of Lorentzian caused by
the uncertainty principle (in Baranger' approach **[4]**),
column "Lorentz" displays FWHM of Lorentzian caused by bigger of
two: either uncertainty principle or Stark effect,
column "Voigt" displays FWHM of Voigh shape of the line,
column "PopUpper" displays population of the upper level, $n_{a,b,Up}/n_{a,b}$,
column "flu" displays the absorption oscillator strength f_{lu} .

In file "*Frames.dat*" the 1st column gives the energy of photons [keV], columns 2-9 display spectral distribution of energy, $FrY_\nu(k)$ radiated by z-pinch in side-on direction during each of eight frames (k = 1, …, 8). All frames are of equal duration "FrL" given in file *Params2.inp*. The last column gives spectral distribution of energy $Y_\nu(t)$ collected during full time of the computation. Spectral edges of the frames **to be defined by user** in file *Params1.inp*. For comparison to the frames of TREX functions $FrY_\nu(k)$, $Y_\nu(t)$ **should be multiplied** by spectral response of the TREX. The units of $FrY_\nu(k)$, $Y_\nu(t)$ are [J/keV/sr].

Files "*CoreEmiAbso.dat*", "*HaloEmiAbso.dat*" display plasma emissivity and absorption coefficient corrected for induced emission in Core and Halo, respectively, both at t = "tiInf" given in file *Params2.inp*. The units are [W/eV/cm^3/sr] and [cm^{-1}].

Column "hvKeV" displays full array of points of photon energy [keV].

Columns 2 - 5 display plasma emissivity: free-bound (i.e. due to radiative recombination), bound-bound (i.e. due to spectral lines), free-free (i.e. radiation of free electrons), total (i.e. the sum of these three).

Columns 6 - 9 display plasma absorption coefficient corrected for stimulated emission: bound-free (i.e. due to photoionization), bound-bound (i.e. absorption in spectral lines), free-free (absorption by free electrons), total (i.e. the sum of these three).

File "*EffSpIns.dat*" displays $J_{v,b}$ (t) taken as 6-direction average in one "representative" point (RP) of each zone at t = "tiInf" given in file "*Params2.inp*". Five of twelve LOSs cross both zones, therefore in each zone $J_{v,b}$ (t) depends on parameters of both zones.

Column "hvEV" shows photon energy [eV],

columns 2 – 6 show spectral inensity of radiatin [W/eV/sr/cm^2] from five directions to RP of the Core. Intensity along the 6th LOS isn't shown because equal to intensity along 5th LOS (column "CoreY").

column "SpInEfCo" shows mean of these six that is $J_{v,\ core}$

columns 8 – 12 show spectral inensity of radiation [W/eV/sr/cm^2] from five directions to RP of the Halo. Intensity along the 6th LOS isn't shown because equal to intensity along 5th LOS (column "HaloY").

column "SpInEfHa" shows mean of these six that is $J_{v,\ halo}$

Files "*PIR_Fe_Core.dat*", "*PIR_Fe_Halo.dat*" display time [ns], $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{Fe,b}$ [cm^{-3}], ratio of the ground state ionization energy in plasma to its table (*single ion*) value. The table value is shown in file Q*SsFe.inp*. The lowering of ionization energy (the lowering of continuum) in plasma is taken in the Ion Sphere approach, see Appendix.

Files *ZpopsFe_Core.dat, ZpopsFe_Halo.dat* display population of the last five ionization stages of **iron** as functions of time along scenario**.** Sum over the stages = 1. Columns of these two files display time [ns], $T_{e,b}$ [keV], $n_{e,b}$ [cm^{-3}], $n_{Fe,b}$ [cm^{-3}], population of Be-like, Li-like, He-like, H-like ions of iron, nuclei of iron.

In file "*PCDs.dat*" the 1st column gives time [ns] along scenario, next three columns give z-pinch side-on radiation power [W] to be shown by three absolutely calibrated diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (those, used in Z shot 1520). The last column gives z-pinch side-on radiation power [W] in full interval ["hvMin" , "hvMax"], no filters.

File "*PCDrespo.dat*" displays spectral response of diamond PCDs with kapton filters of 5-, 10-, 40-mils thickness (PCDs used in Z shot 1520). The 1st column shows photon energy [eV]. Columns 2 – 4 show spectral response of the PCDs in the interval ["hvMin" , "hvMax"]. $0 \leq$ response ≤ 1. Output file "*PCDrespo.dat*" differs from input files "*Respo5milKapPCD. inp", "Respo10miKapPCD.inp", "Respo40miKapPCD.inp"* by number of hν points. In file "*PCDrespo.dat*" the hν points are those of present computation, the response (columns 2-4) is calculated by interpolation between points of the input files.

If users would like to estimate time, t_{CRE}, required for relaxation of level populations to CRE under certain parameters of plasma, he must keep these parameters constant while computing frames with short time step ("*tstep*"). The sequence of frames converges with $t \to t_{CRE}$. The computation should be repeated with 3x, 10x, ... shorter *tstep*, until dependence of t_{CRE} on *tstep* becomes negligible. Keep in mind that t_{CRE} depends on (i) initial distribution of ions over energy levels, (ii) database of levels and cross-sections.

Appendix. Ionization energy of ion a^{q+} in plasma

Widely used models of the reduction of ionization energy in plasma (also known as continuum lowering), $\Delta I_{a,q,b}$, such as Debye-Hűckel, Ion Sphere, Stewart-Pyatt **[4, 9, 10]** ignore few fundamental effects **[11]**. On the other hand, no closed-form expression that accounts these effects; therefore, in present code we use the Ion Sphere model that we modified for plasmas of complex chemical composition.

In plasmas, each free electron moves in collective electric field of other free electrons and ions of different charge and mass. This rapidly-changing collective field complicates trajectories of free electrons. In neutral uniform plasma it results in uniform distribution of free electrons; then **the mean volume per free electron**

$$V_{e,b} \approx 1/n_{e,b}.$$

Due to neutrality of plasma, mean number of free electrons moving through the ion sphere of ion a^{q+} at any time is approximately q, thus the volume of ion sphere of a^{q+} in zone b

$$V_{q.b} \approx qV_{e,b} \approx q/n_{e,b}\,, \qquad (A.1)$$

then radius of the ion sphere

$$\zeta_{q,b} \approx [3V_{q,b}/4\pi]^{1/3} \approx [3q/(4\pi\, n_{e,b})]^{1/3}. \qquad (A.2)$$

If ion a^{q+} is a **solitary one**, it can be treated as a point-like $a^{(q+1)+}$ with one electron bound in potential

$$U(r) = - e\,(q+1)/r\,. \qquad (A.3)$$

Removal of this electron from r to infinity (i.e. ionization of solitary a^{q+}) requires energy

$$I_q = e\,U(\infty) - e\,U(r\,) = 0 + e^2(q+1)/r\,. \qquad (A.4)$$

In neutral plasma, at any instant each ion sphereis traversed by q free electrons. These electrons weaken potential (A.3); on the edge of ion sphere (i.e. on interface of two ion spheres) bound electron does not belong to any of them, thus is free, thus its ionization from $r = \zeta_{q,b}$ does not require energy. In comparison to a solitary ion [*see* (A.4) *at* $r = \zeta_{q,b}$] ionization energy is lower by $e^2(q+1)/\zeta_{q,b}$; in other words, the lowering of ionization energy in neutral plasma

$$\mathbf{\Delta I_{a,q,b}} \approx e^2(q+1)/\zeta_{q,b} = \mathbf{2\,(q+1)\,I_H\,\zeta_0/\zeta_{q,b}}\,. \qquad (A.5)$$

Here we used known relation $2I_H = e^2/\zeta_0$ where ζ_0 is Bohr radius.

Derived $\Delta I_{a,q,b}$ depends on the ion charge and electron density in plasma but does not depend on its chemical and ionization composition, therefore expression (A.5) does not differ (*except factor* $^4/_3$) from result known for identical ions*; numeric factor ~1 depends on assumptions of particular model, *see discussion in Ref.* **[4]**. Comparison of predicted $\Delta I_{a,q,b}$ to experimental data does not prove any model because their predictions (i) differ by less than factor 2, *see e.g. Figs 1, 2 in Ref.* **[12]**, (ii) differ in dependence on plasma density and temperature which in experiments are t, $\boldsymbol{r}$-dependent and have wide error bars.

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* *See expressions (7.42), (7.43) in Ref.* **[4]** *and (10.12) in Ref.* **[13]**.

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