ETS benchmarking and verification
Intermediate report *(ASTRA results)*

On the basis of the previous study the time step $\tau = 10^{-3}$ s and the number of grid points $N_\rho = 101$ has been selected.

Part I. Cylindrical geometry. Consistency and conservation check.
1. Non-coupled equations.

Test I.1.1.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	1 / 1	$P(2,1)$	–	0	0	0
$T_{i,1}$ / 2	1 / 1	$P(2,1)$	–	0	0	0
n_e / 2	1 / 1	$P(2,1)$	–	0	0	0
$n_{i,1}$ / 2	1 / 1	$P(2,1)$	–	0	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Output: $n_{e,i}(\rho,t) - n_{e,i}(\rho,0),\ T_{e,i}(\rho,t) - T_{e,i}(\rho,0).$

Result:
At grid points, all quantities start with being zero in all digits. In course of time evolution they randomly jump with an increment being a multiple of the round-off error

$$\epsilon_{R8} = 2.220446049250313 \times 10^{-16} = \texttt{EPSILON}(\texttt{REAL}(\texttt{KIND} = 8)).$$

There is no clear dependence of this behaviour on the time step or on the grid node number. The overall error (for many time steps) sometimes is added and accumulates, sometimes it does not and stays limited. In this particular case, during the first 10^5 time steps the mismatch was limited to $8\epsilon_{R8}$.
In what follows, if the one-time-step error is commensurable with ϵ_{R8} we shall say that the result is correct to within the machine accuracy.

Test I.1.2. Here $f(\rho,t) = 1 + \sin(t)$

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	1 / 1	$P(2,1)$	–	0	0	0
$T_{i,1}$ / 2	1 / 1	$P(2,1)$	–	0	0	0
n_e / 1	–	–	$P(f(\rho,t),1)$	0	0	0
$n_{i,1}$ / 1	–	–	$P(f(\rho,t),1)$	0	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Comment:
$p_{e,i}$ must stay unchanged.

Output: $p_{e,i}(\rho,t) - p_{e,i}(\rho,0)$.

Result:

The discrepancy $p_{e,i}(\rho,t) - p_{e,i}(\rho,0)$ behaves similar to that of the previous case adding at random time steps multiple of $\pm\,\epsilon_{R8}$. In this case, the error increment changes sign and the overall error stays within $20\,\epsilon_{R8}$.

Test I.1.3.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(2,1)$	–	1	0	0
$T_{i,1}$ / 2	4 / 0	$P(2,1)$	–	1	0	0
n_e / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Comment:

Particles and energy must be conserved.

$$\int_V P(A,B)dV = \frac{A+B}{2}V,$$

$$\int_V P^2(A,B)dV = \frac{A^2-AB+B^2}{3}V$$

Exact solution for n is available

Value of the energy flux in the second column is related to the conductive heat flux q_j ($j=e,i$). Convective heat flux $\Gamma_j T_j$ is discarded, i.e. $c_{1,i}=0$.

Result:

Because zero source and zero flux through the boundary are prescribed the total number of particles and the partial thermal energies should conserve. It means that the integrals

$$\frac{\partial}{\partial t}\int_V n_e(\rho_j,t)dV, \qquad \frac{\partial W_e}{\partial t} = \frac{\partial}{\partial t}\int_V \frac{3}{2}n_e(\rho_j,t)T_e(\rho_j,t)dV$$

and similar for ions should vanish. Numerical implementation of these derivatives should not exceed ϵ_{R8} at each time step. In simulation, a quality of conservation is characterized by the quantity

$$\Delta_{ne} = \sum_{j=1}^{N} n_e(\rho_j,t)V'(\rho_j) \Big/ \sum_{j=1}^{N} n_e(\rho_j,0)V'(\rho_j) - 1 \qquad (1)$$

and so on. The maximum growth rate should be limited by $N\epsilon_{R8}$ that translates to $\Delta_{max} \le \epsilon_{R8}N \approx 10^{-13}t$. In this particular case, Δ_{ne} initially grows at the maximum rate Δ_{max}. As long as the run approaches steady state (in this case, $t \ge 5$ s) the rate drops to zero. In opposite, Δ_{We} does not show the linear growth with N because an increment of Δ_{We} at each time step has a random sign. However, if the grid size N_ρ changes it can happen that Δ_{We} starts to grow linearly while Δ_{ne} oscillates around zero.

Comment:

Although an analytic solution, $n_e^{an}(\rho,t)$, is available for this case it would be not relevant to consider the quantity

$$\sum_{j=1}^{N} n_e(\rho_j,t)V'(\rho_j) \Big/ \sum_{j=1}^{N} n_e^{an}(\rho_j,t)V'(\rho_j) - 1 \qquad (2)$$

in place of Eq. (1). The quantity (2) characterizes an accuracy of numeric scheme. It depends on N_ρ and, in this particular case, is of order $3{\times}10^{-3}$, i.e. by 13 orders of magnitude larger than (1). The value of Eq. (2) should monotonically depend on the time and grid step. The value of Eq. (1) should not. The quantity (1) characterizes the conservation property of a numeric scheme that is the main subject of this section.

Test I.1.4. Discontinuous diffusion coefficient (added in October 2009).
$D(\rho) = 1 + H(\rho - \rho_1), \quad \rho_1 = 1$ m.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(2,1)$	–	$D(\rho)$	0	0
$T_{i,1}$ / 2	4 / 0	$P(2,1)$	–	$D(\rho)$	0	0
n_e / 2	4 / 0	$P(2,1)$	–	$D(\rho)$	0	0
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	$D(\rho)$	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Result:
The behaviour of quantities Δ_{ne}, Δ_{We} and similar is qualitatively the same as in I.1.3. Moreover, the growth rate of Δ_{ne} is by a factor of 2 smaller.

Test I.1.5.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(2,1)$	–	0.1	1	0
$T_{i,1}$ / 2	4 / 0	$P(2,1)$	–	0.1	1	0
n_e / 2	4 / 0	$P(2,1)$	–	0.1	1	0
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	0.1	1	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Comment: At $D \to 0$ the equation degenerates so that only one the two boundary conditions at $\rho = 0$ can be satisfied. Nevertheless, it makes sense to push D in both examples down to zero in order to determine numeric limits and get an idea about residual numerical diffusion of the scheme. For constant v and D the equation $\frac{\partial}{\partial t}\rho n + \frac{\partial}{\partial \rho}\rho\left(vn - D\frac{\partial n}{\partial \rho}\right) = 0$ has a steady state (asymptotic at $t \to \infty$) solution which for parabolic initial distribution $n(\rho, t)|_{t=0} = P(n_0, n_1)$ reads

$$n^{\infty}(\rho) = \frac{n_0 + n_1}{4} e^{v\rho/D} \Big/ g\left(\frac{va_0}{D}\right),$$

with $g(x)$ being $g(x) = \left[1 + (x-1)e^x\right]/x^2$ and $g(x)|_{x\to 0} \approx \frac{1}{2} + \frac{x}{3}$, $g(x)|_{x\to\infty} \approx \frac{1}{x}e^x$. It is seen that the only parameter that influences the analytic result is va_0/D. Numerically, essential parameter is vh/D (so called grid Peclet number), where h is a size of the space grid cell. It is clear that a reasonable result can be expected if $|vh/D| \ll 1$.

Result:

In this example, D has been fixed $D = 0.1$ m^2/s, v was varying. For all runs, the quantities Δ_{ne}, Δ_{We} and similar were conserved with the machine accuracy. All equations show similar behaviour therefore we discuss results for the density only. An accuracy of the numerical scheme has been evaluated as $\varepsilon(\rho) = \left|n_i(\rho, t\to\infty) - n^{\infty}(\rho)\right|/n_i(\rho,\infty)$. This quantity shows practically no dependence on ρ and is given in the table below for different values of v.

v	-5	-4	-3	-2	-1	-.3	-.1	.1	.3	1	2
vh/D	-1	-0.8	-0.6	-0.4	-0.2	-0.06	-0.02	0.02	0.06	0.2	0.4
ε, %	4.5	3.2	2.1	1.3	0.83	0.64	0.21	1.1	2.9	9.5	18.5

Test I.1.6a. Boundary condition – prescribed total current.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 2	1 / 10 MA	$P(0, 2\pi R_0)$	–	$\sigma_{\parallel}^{neo}$	0	0
T_e / 2	1 / 1 keV	$P(2,1)$	–	1	0	Q_{OH}
$T_{i,1}$ / 0	–	–	–	–	–	–
n_e / 1	–	–	$P(2,1)$	–	–	–
$n_{i,1}$ / 1	–	–	$P(2,1)$	–	–	–

Output: Current density, loop voltage, poloidal field energy, Poynting vector, Joule heating.

Result:

In steady state, the central electron temperature saturates at $T_e(0) = 6.83096$ keV The toroidal loop voltage becomes radially independent and takes value $U_{loop} = 0.286386$ V that corresponds to the flux of the magnetic energy $I_{pl}U_{loop,bnd} = 2.863863$ MW. The latter is equal to the Joule heating and the thermal energy flux through the plasma boundary (both are 2.83863 MW). Note that this accuracy is achieved after 1000 s. The total energy of the poloidal magnetic field (inside the plasma volume only) is 198.434 MJ, the total thermal energy of electrons 5.422 MJ.

Test I.1.6b. Boundary condition – prescribed loop voltage.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 2	3 / 0.283863 V	$P(0,2\pi R_0)$	–	$\sigma_{\parallel}^{neo}$	0	0
T_e / 2	1 / 1 keV	$P(2,1)$	–	1	0	Q_{OH}
$T_{i,1}$ / 0	–	–	–	–	–	–
n_e / 1	–	–	$P(2,1)$	–	–	–
$n_{i,1}$ / 1	–	–	$P(2,1)$	–	–	–

Output: Current density, loop voltage, poloidal field energy, Poynting vector, Joule heating.

Result:
This "inversed" problem arrives to a very different solution because of slow thermal instability that occurs for this type of boundary conditions: the electron temperature and the total current either grow unlimited or drop to finite values that are determined by the boundary conditions for the electrom temperature. In this particular case, the central electron temperature is reduced to $T_e(0) = 3.25$ keV, the flux of the magnetic energy into the plasma and the thermal energy outflux are 1.206 MW. The energy of the poloidal magnetic field and the thermal energy of electrons drop to 30.338 MJ and 3.008 MJ, respectively. This steady state is achieved after $\approx 10^4$ s.

Test I.1.7. Non-inductive current drive.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 2	2 / 10 MA	$P(0,2\pi R_0)$	–	$\sigma_{\parallel}^{neo}$	0	(*)
T_e / 2	1 / 1	$P(2,1)$	–	1	0	Q_{OH}
$T_{i,1}$ / 0	–	–	–	–	–	–
n_e / 1	–	–	$P(2,1)$	–	–	–
$n_{i,1}$ / 1	–	–	$P(2,1)$	–	–	–

*) Noninductive current density is set to any radial function normalized in a way that the total non-inductive current is 10 MA, e.g. $j_{ni} = (\pi a^2)^{-1} \times 10^7$ A/m^2.

Result:
The total current should be replaced by a non-inductive current. Loop voltage and the Joule heating drop to zero so that the electron temperature becomes equal to the edge value.

2. Coupled equations. (Cross-equation energy exchange)

Test I.2.1. Similar to I.1.3 but the equipartition term is included on the rhs.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(3,1)$	–	1	0	Q_{ie}
$T_{i,1}$ / 2	4 / 0	$P(1,1)$	–	1	0	Q_{ei}
n_e / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Comment: Particles and energy must be conserved.

Output: Similar to (1) but for total energy contents.

Remark: In the implicit scheme, the total energy should be conserved with a machine accuracy provided all temperature equations are solved simultaneously (matrix inversion). For sequential inversion of each equation a comparable quality of energy conservation can be expected if iterations are enabled.

Result:
Because of the equipartition term only the total energy is conserved here. In the rest, the output has the same features as in the task I.1.3.

Test I.2.2. Similar to I.2.1 but a discontinuous heating term with stepwise time dependence is included $Q_{pulse}(\rho,t) = Q_0\left[H(\rho-\rho_1)-H(\rho-\rho_2)\right]\left[H(t-t_1)-H(t-t_2)\right],$ where $0<\rho_1<\rho_2<a_0, \quad 0<t_1<t_2<T$

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(3,1)$	–	1	0	$Q_{ie}+Q_{pulse}$
$T_{i,1}$ / 2	4 / 0	$P(1,1)$	–	1	0	Q_{ei}
n_e / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Output: Partial energy contents in electrons and ions.

Result:
We select $\rho_1 = 0.5$ m, $\rho_2 = 1.5$ m, $t_1 = 0.2$ s, $t_2 = 0.4$ s, $Q_0 = 0.5\ \mathrm{MW/m^3}$ that corresponds to ≈100 MW of additional heating. If $T > t_2$ then $\int_0^T dt \int_0^{a_0} Q_{pulse}\, dV = 0$ and the energy in both plasma components is conserved with the machine accuracy. The integrals (sums) of type (1) slowly increase with t reaching at maximum $355\epsilon_{R8}$.

Test I.2.3. Particle and energy conservation. Similar to I.2.2 but with non-zero outflux.
Let $Q_i(\rho) = Q_0 \left[H(\rho-\rho_1) - H(\rho-\rho_2)\right]$, $\rho_1 = 0.5$ m, $\rho_2 = 1.5$ m, $q_{i,bnd} = \int\limits_V Q_i(\rho)dV$, $Q_0 = 0.1$ MW/m^3.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / 0	$P(16,15)$	–	1	0	Q_{ie}
$T_{i,1}$ / 2	4 / $q_{i,bnd}$	$P(16,15)$	–	1	0	$Q_{ei}+Q_i(\rho)$
$n_{i,1}$ / 2	4 / 0	$P(2,1)$	–	1	0	0
$n_{i,2}$ / 0	–	–	–	–	–	–

Output: Particle and total energy contents.

Note: Here Q_0 is reduced and the initial temperature increased in order to avoid a negative ion temperature at the plasma edge.

Result:
The ion temperature achieves a steady state within 1 s, electron temperature in 2 s. During the further evolution the total energy contents is limited by $35\epsilon_{R8}$.

Test I.2.4. Particle and energy conservation.
Let $S_i(\rho) = S_0 \left[H(\rho-\rho_1) - H(\rho-\rho_2)\right]$, $\rho_1 = 0.5$ m, $\rho_2 = 1.5$ m, $\Gamma_{i,bnd} = \int\limits_V S_i(\rho)dV$, $Q_i(\rho) = c_{1,i}T_{i,bnd}(\rho)S_i(\rho)$, $Q_e(\rho) = c_{1,i}T_{e,bnd}(\rho)S_i(\rho)$, $D(\rho) = 1 + H(\rho-\rho_3)$, $\rho_3 = 1$ m, $S_0 = 5{\times}10^{18}$ m^{-3}s^{-1}, $c_{1,i} = 5/2$. Note that $q_{i,bnd}$ denotes conductive heat flux.

F value / flag	Bnd. type / value	$F(\rho,0)$	$F(\rho,t)$	D	v	s
ψ / 1	–	–	–	–	–	–
T_e / 2	4 / $q_{e,bnd}=0$	$P(3,1)$	–	1	0	$Q_{ie}+Q_e$
$T_{i,1}$ / 2	4 / $q_{i,bnd}=0$	$P(1,1)$	–	1	0	$Q_{ei}+Q_i$
$n_{i,1}$ / 2	4 / $\Gamma_{i,bnd}$	$P(3,1)$	–	1	0	$S_i(\rho)$
$n_{i,2}$ / 0	–	–	–	–	–	–
n_e / 0	–	–	–	–	–	–

Output: Particle and energy contents.

Result:
The total number of particles is conserved with the machine accuracy, i.e. the quantity (1) is comparable with ϵ_{R8} (in this particular case, gradually increases up to $\leq 500\epsilon_{R8}$). Conservation of energy depends on implementation of the boundary conditions. Namely, the accuracy of the scheme depends on a method (boundary type 3, 4 or 5 in ETS description) of setting edge

conductive flux to zero. For consistent setting the conservation is fulfilled with the machine accuracy. Otherwise, the relative error saturates at the level of 0.05% that is by 13 orders of magnitude larger than the possible best. Nevertheless, adding iterations to the numerical scheme improves the energy conservation. At 2 iterations, the error drops to $\approx 700\epsilon_{R8}$, at 3 and more iterations to $\approx 80\epsilon_{R8}$.

Test I.2.5. "Poloidal" field energy dissipation. For $F = \psi$, $D(\rho, t)$ should be replaced by conductivity $\sigma_{\parallel}^{neo}$.

F value / flag	Bnd. type / value	$F(\rho, 0)$	$F(\rho, t)$	D	v	s
ψ / 2	2 / 10 MA	$P(0, 2\pi R_0)$	–	$\sigma_{\parallel}^{neo}$	0	0
T_e / 2	1 / 1 keV	$P(2, 1)$	–	1	0	$Q_{OH} + Q_{ie}$
$T_{i,1}$ / 2	1 / 1 keV	$P(2, 1)$	–	1	0	Q_{ei}
n_e / 1	–	–	$P(2, 1)$	1	0	0
$n_{i,1}$ / 1	–	–	$P(2, 1)$	1	0	0

Output: Current density, loop voltage, safety factor, poloidal field energy, Poynting vector, Joule heating, energy contents as functions of time and radius.

Results:

At steady state, poloidal energy flux into the plasma coinsides with the total thermal flux from the plasma with the relative accuracy of 10^{-8} being by 8 orders of magnitude worse than the machine accuracy. The magnetic field energy is 198.2 MJ, the total thermal energy 8.097 MJ, the energy [in/out] flux 3.776 MJ, the electron-ion heat exchange 1.71 MJ. Characteristic time (skin time) is about 200 s.

Part II. Stiff transport. (tbd)

A simplified "cylindrical" diffusion equation for a quantity F reads

$$\begin{cases} \dfrac{\partial F}{\partial t} = \dfrac{1}{x}\dfrac{\partial}{\partial x}\left(xD\dfrac{\partial F}{\partial x}\right) + S, \qquad 0 < x < 1, \qquad t > 0, \\ |DF_x(t, x = 0)| < \infty, \qquad F(t, x = 1) = F_1(t), \qquad F_x = \dfrac{\partial F}{\partial x}, \\ F(t = 0, x) = F_0(x). \end{cases}$$

Diffusion coefficient is assumed to have the form $D = D_0 + D_{an}$.
A single equation for the main ion component n_i can be used here in place of F.
The estimate of accuracy should be based on the time behaviour of $F_x = \dfrac{\partial F}{\partial x}$ or D_{an} rather than $F(t, x)$. It would be useful to have an output for the grid quantities

$$Q_f(t, x) = -xDF_x, \qquad Q_s(t, x) = \int_0^x xSdx, \qquad Q_t(t, x) = \frac{\partial}{\partial t}\int_0^x xFdx.$$

Test II.1. Simple model.
Stiff transport is described by $D_{an} = D_1 \max(0, -F_x - \eta_{cr})$ that switches on a stiff transport once $|F_x|$ exceeds η_{cr}. The following input parameters are proposed

$$F_0 = 0.1, \qquad D_0 = 0.1, \qquad \eta_{cr} = 1,$$
$$F_1 = 0.1, \qquad D_1 = 1, \qquad S = 1.$$

Test II.2. Stiff transport + transport barrier.
$D_{an} = D_1 \min[\max(0, -F_x - \eta_{cr}), 0.07/(-F_x - \eta_{cr})$. The added correction suppresses the stiff transport in the range where $|F_x| > \eta_{cr} + \sqrt{0.07}$.
The input parameters are the same as in II.1 except for $S = 1 + P(1, 0)$. This change restricts an extension of the transport barrier to $0.525 < \rho/a_0 < 0.75$.

Test II.3. If a special scheme is implemented to treat stiff transport then two additional runs should be performed for a non-stiff transport $D_1 = 0$. One run should use the "stiff" numeric scheme, another a regular scheme. The aim is to evaluate distortions introduced by the stiff scheme to a non-stiff transport.
