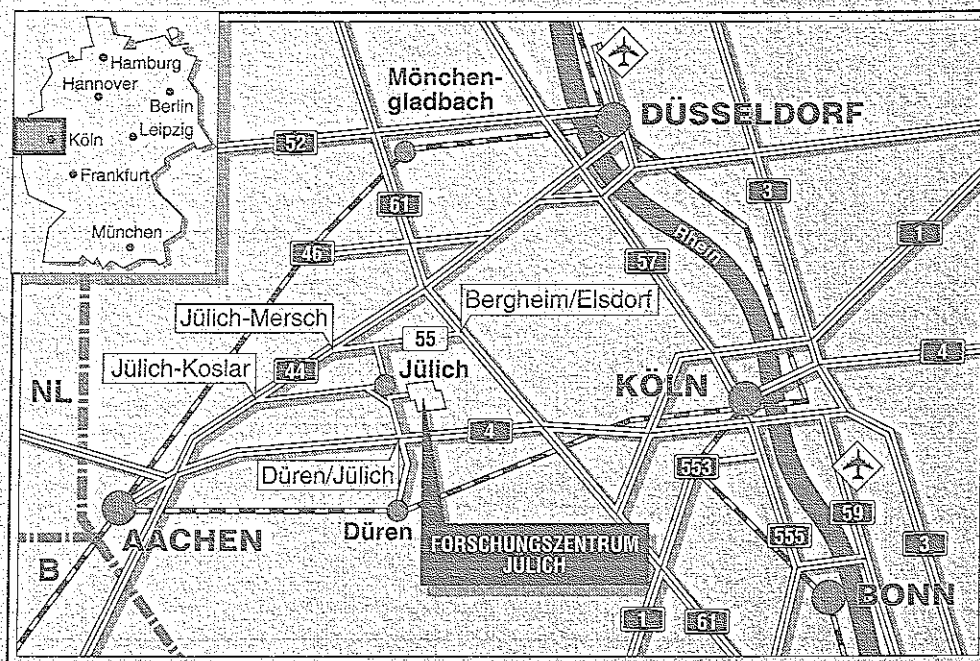


Institut für Plasmaphysik
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Recycling source terms for edge plasma fluid models and impact on convergence behaviour of the BRAAMS "B2" code

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These are the various signs of the
presence of the Lord in the world
and in the hearts of men. The
Lord is with us in the world
and in the hearts of men.

THE LORD IS WITH US

THE LORD IS WITH US
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THE LORD IS WITH US

Abstract

Predictive simulations of tokamak edge plasmas require the most authentic description of neutral particle recycling sources, not merely the most expedient numerically. Employing a prototypical ITER diverter arrangement under conditions of high recycling, trial calculations with the "B2" steady-state edge plasma transport code, plus varying approximations of recycling, reveal marked sensitivity of both results and its convergence behaviour to details of sources incorporated. Comprehensive EIRENE Monte Carlo resolution of recycling is implemented by full and so-called "short" intermediate cycles between the plasma fluid and statistical neutral particle models. As generally for coupled differencing and stochastic procedures, though, overall convergence properties become more difficult to assess. A pragmatic criterion for the "B2"/EIRENE code system is proposed to determine its success, proceeding from a stricter condition previously identified for one particular analytic approximation of recycling in "B2". Certain procedures are also inferred potentially to improve their convergence further.

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1. Introduction

Reliable computational studies of conditions in tokamak edge regions require consistent and detailed descriptions of both plasma transport and volume sources due to interactions with recycled neutral particles. In a large next-step device such as ITER, pulse length and edge plasma collisionality are expected to be sufficient to permit a steady-state, fluid representation of plasma behaviour, as embodied for axisymmetric systems in the two-dimensional BRAAMS "B2" code^{1,2}. This provides a primary treatment, on a basis of classical transport along magnetic field lines, and anomalous relations of essentially empirical form normally between flux surfaces. Simultaneously, however, recycling at target plates is expected to be very high, so that dependent source terms are very strong, locally even dominant. Hence a treatment of at least comparable detail is clearly also demanded for accompanying neutral particle effects.

Initial approximations of recycling sources in BRAAMS calculations were based on certain simplified, analytic models. A first, so-called "minimal" model² addressed only reionization of atomic particles, with fixed, radiatively-modified electron energy loss and ion dilution cooling. A subsequent, more sophisticated treatment due to Hotston³ accommodated various additional effects, notably a number of major molecular channels, but still only crudely allowed for neutral particle motions across magnetic surfaces, or for diffusion via charge-exchange events. While these computationally simple and fast approaches could yield a very high degree of consistency with plasma transport, therefore, they were disadvantageously lacking in *detail*. An alternative approach giving a virtually exact description via Monte Carlo synthesis of neutral particle behaviour, such as in the EIRENE code⁴, is thus being adopted[†]. In this case, having complete but computationally expensive *detail*, the complementary problem now occurring is how to achieve a similar level of *consistency*.

Precise features of recycling source distributions are indeed seen to exert a pronounced influence on plasma solutions. In a supplementary Fig.24, this is illustrated for equivalent "B2"/Hotston and "B2"/EIRENE calculations on an ITER-related divertor system described fully later. A Hotston treatment typically imposes pumping by non-unit reflectivities $\mathcal{R}$ for ions impacting on target surfaces, and a first EIRENE instance replicates such a condition by identical target albedoes for impinging particles. Note one essential difference between these two neutral particle approaches is that the Hotston approximation excludes their possible re-impact on a plate, with a corresponding fractional absorption again, and also forces their complete reionization³ within the calculation domain. Since EIRENE already lifts both restrictions, for the latter by permitting neutral particle escapes back into the core if arrived at, associated results immediately differ concerning the level of recycling derived, even for fixed $\mathcal{R}$ values. An exact definition of recycling flux amplification $\mathcal{F}$ is again given subsequently. More particularly, while plasma total scalar pressure facing the outside lower target is very similar for both cases,

[†]Coupling of the EIRENE and "B2" codes was developed at KFA Jülich under Euratom/NET contract, 1988-1990 — see final report on NET contract 428/90-8/FU-D,

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Most extensive application to present machines has been performed by R Schneider, J Neuhauser *et al*, IPP Garching — see initially ref.8.

The second part of the document provides a detailed overview of the accounting system used by the organization. It describes the various components of the system, including the general ledger, subsidiary ledgers, and the trial balance. The document also explains the process of recording transactions and the importance of double-entry bookkeeping.

The third part of the document discusses the various methods used to calculate the cost of goods sold. It compares the first-in, first-out (FIFO) method with the last-in, first-out (LIFO) method and explains the advantages and disadvantages of each. The document also discusses the importance of accurate cost calculations for determining the gross profit margin.

The fourth part of the document discusses the various methods used to calculate the depreciation of fixed assets. It compares the straight-line method with the accelerated methods and explains the advantages and disadvantages of each. The document also discusses the importance of accurate depreciation calculations for determining the net book value of the assets.

The fifth part of the document discusses the various methods used to calculate the income tax expense. It compares the accrual method with the cash method and explains the advantages and disadvantages of each. The document also discusses the importance of accurate income tax calculations for determining the net income of the organization.

underlying properties like electron temperatures are quite distinct. Much higher values obtained with EIRENE would actually be a crucial factor regarding practicality of the design.

In addition signally to more realistic neutral particle transport, EIRENE also allows an improved representation of pumping, by substituting partial absorption of neutral particles at a plausible duct entrance. As revealed in Fig.24, this results in an extra slight modification of the plasma, but still close to the preceding EIRENE outcome, and removed from that with Hotston sources. Further emphasis is provided in Fig.25, where each plasma flow field is depicted over a projection of the outside lower divertor sector. This element of scrape-off layer (SOL) solutions would again affect a crucial capacity of the divertor to exhaust impurity ions, and is moreover a fine measure of distributed behaviour. Similarity of both EIRENE cases is again evident, plus their joint departure from the Hotston result.

It therefore becomes clear that significant changes in simulations arise from advancement from Hotston to EIRENE recycling itself, but not from subsidiary alterations in boundary conditions of target surface to duct entrance pumping. We consequently concentrate in subsequent discussions exclusively on the latter formulation, the purpose in adopting EIRENE being to obtain the most authentic statement available. Furthermore, not only final states are sensitive to particular source treatments, but also *approach* or *access* of the model to them. In other words, important repercussions emerge too for the fundamental technical issue of code *convergence*, governing achievement of required consistency.

In a recent thorough, systematic investigation of numerical behaviour of the "B2" code with Hotston recycling, still for conditions relevant to the ITER divertor, the importance of ensuring valid convergence of its iterative relaxation to steady state was plainly indicated⁵. Here this denotes an exponential decline of unsteady terms in its underlying plasma transport equations^{1,2}, or equivalently in balance errors of global quantities such as particle content and power through-put⁵. Key features of divertor "solutions" were shown not to be correct in the absence of such a signature⁵. The argument has to be considered, then, with regard to separate performance of "B2" for similar conditions, but involving instead EIRENE determination of recycling sources[†]. An outer "cycling" technique between "B2" and EIRENE is employed to seek overall convergence, and so consistency, with certain implicit revision of source terms according to the EIRENE atomic reaction data through intervening "B2" internal iterations⁶. Attention centres on an observation that typically relaxation of convergence measures does not seem to exhibit clear exponential trends. Possible implications for validity obviously have to be decided.

An aspect of "B2" numerical behaviour not addressed in the former study (ref.5) was possible *specificity* of the characteristics found to the particular model of recycling source terms invoked, namely the Hotston analytic approximation. In other words, they might not define generic performance, but only an idealization, with other modes of behaviour being available for different representations. Under these circumstances, some component at least of distinct conduct when coupled with EIRENE could be attributable merely to alterations in form relating to its derived sources, rather than signifying numerical

deficiencies. Evidently it is necessary at least to eliminate such a possibility from the discussion, in order to isolate any genuine numerical problems. The exercise is pertinent to the goal, noted above, of finding results incorporating the most *physical* description of recycling, furnished by EIRENE, rather than just the (probably distinct) most well-behaved numerically.

In this report, convergence of "B2" calculations for a prototypical ITER divertor are first contrasted, using those alternative treatments of recycling sources already mentioned: (a) "minimal" and (b) Hotston analytic models; (c) EIRENE. Conditions are otherwise kept exactly identical in corresponding cases. Respective source distributions are compared in detail, and susceptibility of behaviour to small relative changes between them examined. Then considering more specifically the technique[†] for linking "B2" and EIRENE as developed at KFA Jülich since the late 1980s, now widely used also in other fusion laboratories, a number of possibilities for its further improvement are suggested. Points raised should have general applicability to any fluid plasma / Monte Carlo neutral particle model under development. Finally, the connotations must be considered with regard to assessment of valid convergence in most realistic "B2" simulations coupled to EIRENE. We infer a pragmatic way in which this might be judged.

2. ITER divertor configuration

Calculations are performed for a poloidal magnetic divertor geometry and boundary conditions representative of expectations for the ITER tokamak. A cross-section of the discretized computational domain is depicted in physical co-ordinates in Fig.1, together with its numerical arrangement. Recall that for an axisymmetric system of two-dimensional plasma transport parallel and normal to magnetic field lines, boundaries of discrete cells⁷ are defined by magnetic flux (ψ) surfaces and contours everywhere orthogonal to them (ie aligned with $-\nabla\psi$). All versions of the BRAAMS model are currently framed with respect to such curvilinear but *orthogonal* co-ordinates^{1,2}. In particular, target plate sections are consequently approximated here merely by flux-orthogonal contours passing through their prescribed strike-point positions.

An exactly up-down symmetric double-null system is supposed, so that one half only need be modelled. Thus asymmetry of pumping from the divertor chambers, as is probable in practice, is for instance neglected. Special attention has been given to tailoring resolutions of the discretization to anticipated small scale-lengths of eventual solutions in those regions adjacent to the separatrix and in front of target plates⁷. The last three cells facing inside targets and four facing outside targets are each about 1 mm in extent *along the field*, for example, while the first three rows in both inside and outside SOL branches have transverse widths of roughly $\frac{1}{2}$ mm at the equatorial (up-down symmetry) plane[¶].

In addition to inside and outside SOL's, an annulus of closed flux surfaces interior to the separatrix, and divertor private flux regions, are also included. The former permits an innermost boundary condition denoting connection with the core plasma to be imposed on a surface of more certain poloidal uniformity. Properties at the separatrix are then determined through the transport model itself. A corollary of this treatment, however, is that there exists no continuous transformation of the physical structure into the topologically rectangular computational domain^{1,2} of BRAAMS. A required discontinuous mapping is indicated in Fig.1 by alphabetical labels, disclosing its numerical grid "cuts" $B \rightarrow B'$; $E \rightarrow E'$ needed to separate physically disjoint zones. Presently these cuts are defaulted simply to isolating barriers, forcing artificial conditions of zero fluxes on their faces. In fact, considerable progress⁸ has been made recently in removing this restriction and permitting continuous fluxes between physically contiguous surfaces $B \equiv E'$; $B' \equiv E$. Note that such an improvement here is itself less reasonable without simultaneously accounting for impacts of real oblique target sections, and asymmetric pumping mentioned above.

A perimeter of the system is defined by outermost SOL surface $A' \rightarrow C'$; $D' \rightarrow F'$. In other words, no surrounding vessel wall is included. For "minimal" and Hotston analytic recycling models this is incidental, but for EIRENE simulation of recycled neutral particles the SOL boundary consequently enters as a reflecting barrier. In all cases, actual recycling is initiated only from the explicitly orthogonal target surfaces $A \rightarrow A'$ (T_{IN}); $F \rightarrow F'$ (T_{OUT}). As hinted in §1, analytic and Monte Carlo neutral particle descriptions also differ importantly in representations of pumping: for the former, a fixed fraction $(1 - \mathcal{R})$

[¶]Note an approximate refinement procedure involved⁷ incurs some departures from orthogonality, most prominently quite close to the X-points.

of *target ion* fluxes is removed by imposition of a constant reflection coefficient $0 \leq \mathcal{R} \leq 1$; for the latter, a fraction of *neutral particles* impinging on that portion of the outside divertor *boundary* $G \rightarrow F'$ is removed, again by a non-unit albedo, corresponding to some set pumping speed. This arc matches a possible location of a real duct entrance.

Plasma specification

The so-called “standard” BRAAMS “B2” edge plasma transport model assumes pointwise quasi-neutrality and ambipolarity^{1,2}, ie electric currents are identically excluded. Furthermore, no cross-field plasma drifts within flux surfaces (ie parallel to $\mp(\mathbf{B} \times \nabla\psi)$) are admitted, so that components parallel to $\mathbf{B}$ and $-\nabla\psi$ completely specify the flow field.

A single average ion species of mass number 2.5 and unit charge is considered ($Z_{\text{EFF}} \equiv 1$), symbolizing a pure mixture of 50% ^2H and 50% ^3H . This approximation facilitates isolation of basic features of convergence behaviour, while omitting physically important radiation sinks due to impurities.

Transport coefficients

Conventional classical expressions^{1,2} are employed for each coefficient parallel to magnetic lines of force. In particular, negligible flux limitation^{1,2} of electron thermal conductivity is supposed.

Anomalous, or phenomenological, relations are assumed for coefficients referring to transport between magnetic surfaces, as detailed in Table 1.

Table 1. Transverse transport coefficients

$(1/(m_i n_i)) \times \text{ion viscosity}$	$(\text{m}^2 \cdot \text{s}^{-1})$	$\eta_y^i/(m_i n_i)$	0.2
electron thermal diffusivity	$(\text{m}^2 \cdot \text{s}^{-1})$	χ^e	2.0
ion thermal diffusivity	$(\text{m}^2 \cdot \text{s}^{-1})$	χ^i	0.667
$\nabla_y n_i$ -driven particle diffusion	$(\text{m}^2 \cdot \text{s}^{-1})$	D_y	0.667
particle inward-pinch velocity	$(\text{m} \cdot \text{s}^{-1})$	v_y	0.

Boundary conditions

A fixed set of governing boundary conditions is also applied in all cases, except for alternative implementations of pumping between analytic and EIRENE recycling treatments as related above, and variations in associated reflection coefficient $\mathcal{R}$ of targets for the former. Where indicated below, imposition is according to the “strong”, or dominant source term, prescription of Patankar⁹, which forces always precise adherence to specified values.

- Interface with core plasma (grid “South” edge $B' \rightarrow C$; $D \rightarrow E$)

density	:	value $n_{i\text{SOUTH}} = 3.9 \times 10^{19} \text{ m}^{-3}$	(strong)
parallel momentum	:	zero parallel flow	(strong)
electron energy	:	inside ($B' \rightarrow C$) power input 8.85 MW	} distributed poloidally uniformly
	:	outside ($D \rightarrow E$) power input 34.8 MW	
ion energy	:	inside ($B' \rightarrow C$) power input 2.95 MW	} distributed poloidally uniformly
	:	outside ($D \rightarrow E$) power input 11.6 MW	

- Perimeter (grid “North” edge $A' \rightarrow C'$; $D' \rightarrow F'$ and private flux edges $A \rightarrow B$; $E' \rightarrow F$)

density	:	zero source	
parallel momentum	:	zero shear	(strong)
electron energy	:	[†] pedestal temperature of 2 eV	(strong)
ion energy	:	[†] pedestal temperature of 2 eV	(strong)

- Targets – Bohm sheath conditions for oblique field line incidence¹⁰ (grid “West” edge $A' \rightarrow A'$ (T_{IN}) and “East” edge $F \rightarrow F'$ (T_{OUT}))

density	:	zero parallel gradient	(strong)
parallel momentum	:	sonic parallel flow $c_s = \sqrt{\frac{T_i + T_e}{m_i}}$	(strong)
electron energy	:	power density $\beta_e n_e c_s \left(\frac{B_0}{B}\right) T_e$ ($\text{W} \cdot \text{m}^{-2}$); $\beta_e = 4.8$	
ion energy	:	power density $\left\{ \frac{1}{2} m_i n_i c_s^2 + \frac{5}{2} n_i T_i \right\} c_s \left(\frac{B_0}{B}\right)$ ($\text{W} \cdot \text{m}^{-2}$)	

[†]These constraints are sometimes replaced instead by zero sources, where noted below.

Convergence measures

A prime objective of SOL plasma calculations for a long-pulse device such as ITER is to identify unambiguous steady states, in the case of BRAAMS applications as solutions of a boundary-value formulation^{1,2}. By definition, these are manifested as cases for which unsteady terms vanish asymptotically through its iteration procedure – at least to the limits of technical methods. Convergence to this situation in “B2” is monitored by particle, electron energy and ion energy residuals, each having dimensions of frequency, and related to normalized moduli of their corresponding unsteady terms over the computational mesh, excluding grid cuts.

Subsequent plots of these quantities show their evolution versus a cumulative iteration “time” equal to the sum of values of preceding iterative “time-steps”. Here it should be recalled that the BRAAMS “time” variable acts chiefly as a numerical under-relaxation argument of inertial type^{1,2}, and that additional under-relaxation parameters are also applied to each sequential correction of transport balances. These parameters are set to $\frac{1}{2}$, except where discussed below.

3. Convergence behaviour

3.1 Outline of the discussion

A stringent definition of perfect convergence of a BRAAMS “B2” calculation could be taken as pure exponential decline of its balance equation residuals, as described above, through its numerical iteration procedure^{1,2}. Unequivocally, such a criterion would select clear, steady-state solutions. Acquisition of this ideal signature is certainly possible, and for example is illustrated for the ITER configuration introduced above, in Fig.2. Here Hotston analytic treatment of recycling sources is used, together with zero-source boundary conditions for electron and ion energy equations on the perimeter. For reference later, the final state obtained will be designated H_1^{zs} . It should also be noted that a time-step size of 10^{-5} s is employed, and inside and outside target reflection coefficients $\mathcal{R}_{IN,OUT}$ are assigned high-recycling regime values of 0.997; 0.9985 respectively.

An accompanying measure of convergence is provided by inside and outside divertor values of ion flux amplification $\mathcal{F}_{IN,OUT}$, defined as the ratios of target fluxes $\Gamma_{TIN;TOUT}$ (s^{-1}) to those incoming $\Gamma_{SOUTHIN;SOUTHOUT}$ (s^{-1}) through respective portions of the innermost interior surface ($B' \rightarrow C$; $D \rightarrow E$). Considering for instance $\mathcal{F}_{OUT} \equiv \Gamma_{TOUT}/\Gamma_{SOUTHOUT}$, if no recycled neutral particles escape from the computational outside divertor domain, then it follows that :-

$$\Gamma_{SOUTHOUT} = (1 - \mathcal{R}_{OUT})\Gamma_{TOUT} \Rightarrow \mathcal{F}_{OUT} = \frac{1}{1 - \mathcal{R}_{OUT}} = 666.67$$

Recall that egress through the grid “South” edge, back into the core plasma, would actually be the only means of escape for neutral particles in this case (grid cuts serve also as impenetrable barriers for them). In fact, in solution H_1^{zs} amplification $\mathcal{F}_{OUT}$ is found to be 667.10. Similarly, for any individual cell of volume V_{cell} (m^3) within the discretized grid, a local ion balance error may be constructed :-

$$\epsilon_{cellIN,OUT} \equiv \frac{1}{\Gamma_{SOUTHIN,OUT}} \int_{V_{cellIN,OUT}} (S_n - \nabla \cdot \Gamma) dV, \quad (1)$$

where S_n ($m^{-3} \cdot s^{-1}$) is entire ion source rate and Γ ($m^{-2} \cdot s^{-1}$) is (axisymmetric) ion flux density vector. Such a quantity should of course everywhere be identically zero in a perfect steady state, but again in H_1^{zs} its greatest magnitude in any outside-region mesh cell is found to be 2.03×10^{-5} .

Both measures $\mathcal{F}$; ϵ_{cell} are very sensitive functions under prescribed conditions of high recycling, since only a very small change in Γ_{SOUTH} can induce a very large one in Γ_T . Accordingly in ϵ_{cell} , amplified fluxes contributing in Γ , and thence via recycling in S_n , can be hundreds of times larger in magnitude for cells close to target boundaries than the denominator Γ_{SOUTH} . Accurate achievement of expected and near-zero figures respectively are each therefore strong indicators of a good steady state. Together with a pure exponential decay of its balance equation residuals, then, final state H_1^{zs} must by any reasonable standards be deemed a well-converged, steady result. This type of categorical approach to obtaining valid BRAAMS conclusions is, for example, as subscribed to in ref.5.

In contrast, final traces of residuals when EIRENE resolution^{4,6} of recycling sources is involved are exemplified in Fig.3. Here zero electron and ion energy sources are again imposed on the perimeter, together with duct entrance pumping of neutral particles as explained above. A number of "B2"/full EIRENE cycles are shown, with intervening sets of "short" cycles⁶, during which neutral distributions are rescaled and plasma sources recomputed according to identical reaction data (see §4 below for a fuller account of this procedure). Associated time-steps here are 4×10^{-6} s. Up to a certain ceiling, numbers of "short" iterations before a next full EIRENE call are determined automatically⁶, by setting limits for maximum changes allowed globally in last full EIRENE particle and energy sources. When these would be exceeded, in other words, a full Monte Carlo calculation is newly executed.

Cycles displayed in Fig.3 are actually preceded by many previous ones: initially very brief with strong adjustment of conditions; eventually over which the number of "short" cycles tends gradually to increase, plus the levels to which residuals fall through them tend to decrease. For those last three cycles presented, 5000; 5000; ~ 1300 "short" iterations respectively are performed (5000 being the set ceiling value). Corresponding plasma states after each set are denoted E_{III}^{zs} ; E_{IV}^{zs} ; E_V^{zs} . At each full EIRENE intervention, a significant, repetitive perturbation is evident of small residuals established during the preceding stage. Its following set of "short" cycles then tends to recover from this disturbance, at first rapidly, and subsequently more slowly. Such a pattern tends to repeat itself indefinitely.

Generality of this trend is supported by a wholly similar conclusion, shown additionally in Fig.26, to the separate "B2"/EIRENE calculation cited in §1, namely with Hotston-like, target-surface albedoes replacing duct entrance absorption. Again preliminary cycles lead finally to those long, periodic ones depicted.

The question fundamentally to be decided, therefore, is whether states like E_{III}^{zs} ; E_{IV}^{zs} ; E_V^{zs} might be considered to be converged in a sense similar to that of analytic recycling result H_I^{zs} . Investigation of apparently contrasting behaviour in Figs.2&3 motivates our following examination of BRAAMS "B2" performance for variations in details of recycling sources.

3.2 Perturbation of relaxed state

Even within the "ideal" case of relaxation to plasma H_I^{zs} in Fig.1, it is possible to discern a brief preliminary phase of very rapid amendment, before a transition at $\sim 0.01 \rightarrow 0.03$ s to a persistent stage of slower, but uniform, exponential convergence.

This tendency is revealed more clearly in Fig.4, where the consequence of applying a perturbation to well-converged state H_I^{zs} is traced. A trial disturbance is exerted by switching energy boundary conditions on the perimeter from zero sources to pedestal temperatures of 2 eV, as cited in §2 above. No other conditions (including time-step size) are altered. Now there is a manifest initial fast adjustment of residuals, succeeded by a return to exponential decline at levels and rates, at least as functions of cumulative iteration time, similar to those before (cf Fig.2). End plasma state here is designated H_I^{tp} .

Such a feature does seem reminiscent of evolution of residuals through short-cycle iterations, after full EIRENE calls, in the alternative source model calculation of Fig.3. In other words, each full EIRENE intervention may effect some repetitive perturbation of an essentially relaxed plasma – for the short-cycle representation of recycling sources. This departure is then quickly recuperated, before an effectively asymptotic convergence is restored. We discuss this possible interpretation further below.

3.3 Monotonicity

When some boundary-value problem is solved numerically by an iterative method, as for instance^{1,2} in the BRAAMS code, at least three types of potential behaviour should be discriminated :-

- i) clear convergence, with exponentially small errors,
- ii) clear divergence, with arbitrarily growing errors,
- iii) no explicit convergence or divergence, with errors exhibiting no trends towards either diminishing or increasing values.

In the last indeterminate contingency, a failure of the method could still be signalled, or conceivably access by it to some underlying feature of the model problem, which may both inhibit convergence and carry some other relevance. In our case of concentration on steady states at least, as proposed above, this condition would by definition be a failure so to conclude, and could more simply be reduced to an exclusion supplementing category ii).

It was demonstrated in ref.5 that with Hotston analytic source terms, selection of an inappropriately large time-step size for a given problem can lead to “B2” behaviour of preceding type iii). Unambiguously proper relaxation i) could generally be restored by reducing the time-step below a certain level, which itself may be difficult to anticipate in any particular situation⁵. An equivalent deficiency does not seem to be affecting “B2”/EIRENE evolution monitored in Fig.3, however. Recall time-steps through intermediate “short” iterations here are 4×10^{-6} s. A complementary calculation is plotted in Fig.5, in which conditions are identical except for (a) an increase of later short-cycle time-steps, where indicated, to 4×10^{-5} s, and (b) a small simplification of actual short-cycle treatment of recycling sources. This latter distinction is again examined in more detail below. Immediately, though, production of regular oscillatory residuals during last two long sequences of “short” cycles can be discerned. Note that these failures of residuals to decrease occur whilst global changes of last EIRENE sources never-the-less remain within fixed criteria of the automatic recourse to full EIRENE calls⁶, so that mounting numbers of “short” iterations are permitted (~ 600 ; 1000 respectively). Moreover, fractional errors in global particle and total energy balances⁵ over the outside divertor region (DFF/D') remain small, or even still diminishing for the former, as seen in Fig.6. These final convergence measures are also defined precisely in subsequent remarks.

Plasma states after the last two sets of “short” iterations in Fig.5 are labelled E_1^{zs} ;

E_{II}^{zs} respectively. They hence appear to typify lack of convergence owing to an excessive time-step value, but now with EIRENE sources, comparable to that analysed in ref.5. Elimination of such a difficulty is illustrated in Fig.7 by a continuation from E_I^{zs} , unmodified except for time-steps being limited to 4×10^{-6} s. Manifestly residuals no longer oscillate, but decline, to magnitudes substantially lower than before in Fig.5. They are ultimately arrested, in fact, by a numerical failure of a different nature – namely a tendency locally to generate negative ion temperatures. This unphysical fatality appears quite frequently in a variety of “B2” applications (even being possible with “minimal” recycling supplying only dilution cooling of ions²), and motivates that modification of the short-cycle sources model already referred to as being incorporated into “B2”/EIRENE cycles in Fig.3. A fuller commentary, as mentioned, is given later. The series of cycles in Fig.3, leading then to states E_{III}^{zs} ; E_{IV}^{zs} ; E_V^{zs} , is also a continuation from plasma E_I^{zs} , however, with the smaller time-steps and improved short-cycle recycling noted.

Apparent absence of time-step complications from revised cycles in Fig.3 further supports the previous proposition of their correspondence to well-converged results.

One other point concerning monotonicity of decay of residuals should also be observed. In Fig.8 a calculation matching that of Fig.2 is reproduced, retaining zero-source boundary conditions at the perimeter for both energy equations, but substituting instead the “minimal” analytic model² of recycling sources. Time-steps are reduced to 4×10^{-6} s, while inside and outside target reflection coefficients of 0.997; 0.9985 are preserved, and in particular the identical starting plasma (at iteration time 0) to that in Fig.2 is used. Approximately exponential fall-off is again eventually achieved, yielding final plasma M_I^{zs} , but a clear excursion of residuals can in this case be seen to occur after $\sim 4 \times 10^{-3}$ s. This fluctuation develops abruptly in an already decreasing trend, and can only be related to differences in details of source terms between Hotston and “minimal” analytic treatments. Note state M_I^{zs} is still markedly less well converged than its counterpart H_I^{zs} , as confirmed by outside-region figures for flux amplification $\mathcal{F}_{OUT} = 787.15$ and greatest local ion balance error (cf (1)) $|\epsilon_{cell_{OUT}}|_{max} = 2.90 \times 10^{-3}$.

A first small indication is thus given of a potentially very important sensitivity to precise features of recycling representations. Since alterations of just such a character are involved in a graduation from Hotston analytic to EIRENE Monte Carlo estimation, there are obvious possible connotations. We focus attention on this issue in following sections.

3.4 Ion source distributions

Comparing instances presented above (and summarized finally in Table 2), it will be appreciated already that larger BRAAMS time-steps are employed in conjunction with Hotston recycling (H_I^{zs} ; H_I^{tp}) than with either EIRENE (E_{III}^{zs} ; E_{IV}^{zs} ; E_V^{zs}) or “minimal” (M_I^{zs}) alternatives. In ref.5, a size up to 4×10^{-5} s is used successfully in “B2” plus Hotston solutions of ITER-relevant conditions, even though this is beyond the permissible range of equivalent calculations coupled to EIRENE (or actually with “minimal” recycling as well), as evidenced by foregoing case E_I^{zs} ; E_{II}^{zs} . This “anomalously” good stability of “B2” with Hotston sources, by comparison with both Monte Carlo and simpler analytic treatments, has been reported before in an earlier study¹¹, but remains yet to be resolved.

Susceptibility of “B2” convergence behaviour to *details* of source terms, as mooted above, suggests some key distinctions could perhaps obtain in Hotston distributions. One aspect specific to Monte Carlo sources, for example, is their inclusion always of some level of statistical noise, although of course “minimal” analytic expressions would not be so affected. To illumine possible factors, however, ion source rates *per cell* (ie $S_n V_{\text{cell}} \text{ s}^{-1}$) according to each model are compared in Fig.9 for a common plasma background, namely state H_1^{25} . In other words, then, only instantaneous source functions are computed with EIRENE and “minimal” procedures, so that they do not constitute converged, consistent conditions of sources and plasma, as H_1^{25} does with Hotston terms. To facilitate examination, profiles in labelled grid rows ($-\nabla\psi$ or σ_y increments) of the outside divertor sector (DFF'D') are plotted in Fig.9 against longitudinal cell index (B_y or σ_x direction), which expands physically very small cells containing large source rates adjacent to target surfaces. Moreover since interest centres primarily on profile *shapes* rather than absolute numbers, distributions from each model are normalized by the maximum value (s^{-1}) achieved by any one of them within the chosen domain.

All three treatments can be seen reasonably to agree on dominant source rates close to the target, except that “minimal” values tend to be somewhat too low immediately before it. In effect, this approximation tends to generate too many ions at its distribution peak a canonical reionization distance away, and also facing the target towards the outermost boundary ($iy = 31$).

Furthermore, there is generally fair agreement on ranges, or decay of each distribution, away from the target – other than in one crucial respect. Clearly Hotston recycling fails to reproduce the *long-range* contributions (lower ix positions) within both SOL and even interior plasma regions. These arise from far penetration of recycled neutral particles through outer SOL plasma channels of low density and temperature, and so long mean-free-path lengths, followed by deep redistribution inwards across magnetic surfaces. With EIRENE, such cross-field motion is associated with authentic charge-exchange events. It also seems to be mimicked remarkably well in the “minimal” sources, which even marginally exaggerate incursion to farthest interior cells (lowest ix , iy data). Note that the Hotston distribution has an inverse over-estimate of source rates in outermost plasma zones, since these are not correspondingly depleted by preceding inward relocation.

An additional point is that “minimal” recycling evaluates sources over a plasma sector explicitly defined by certain parameters assigned internally². Here these have been chosen to allow an unrestricted scan over the whole physical space, permitting for instance former excess transport of neutral particles into interior elements. This process has rather been prohibited in all other “minimal” calculations reported, eg reaching solution M_1^{25} , by curtailing its scan at the separatrix between divertor throats. Also lastly, those SOL cells lying in the projected grid-cut columns ($ix = 34$ in Fig.9) are physically spurious, and consequently are excluded by EIRENE, which always returns zero source rates within them.

One distinguishing feature of the Hotston model, therefore, is its reduced degree of neutral particle transport across flux surfaces, so that filling-in of sources at long range is omitted. Whether this could underlie its superior stability, of course, has yet to be

determined. Only ion sources have been examined above, and it is clear that differences might be expected too in accompanying plasma energy sinks, owing to widely disparate sets of reaction channels and their representations respectively encompassed. Nevertheless, spatial ranges of energy sinks at least may largely remain close to those suggested by foregoing ion sources. Relatively greater *locality* of Hotston recycling could be its conclusive characteristic.

The propensity for long-range recycling behaviour naturally may lead to somewhat different plasma solutions, even given a fixed set of boundary conditions. An example is provided by previous states H_I^{zs} , M_I^{zs} , which it will be recalled are *exact* equivalents for Hotston and “minimal” approximations. Their respective ion source rates (s^{-1}) are contrasted in Fig.10, now mapped simultaneously over grid cell indices ix, iy in the outside divertor branch (DFF'D'), and once more normalized by the greatest rate (s^{-1}) achieved by either one. Contours are depicted at successive decimal orders of magnitude below the peak, ie 10^{-1} ; 10^{-2} ; ...; 10^{-6} . It is evident that not only long-range sources are different, but unlike the first test in Fig.9, also individual maxima no longer coincide. Hence adjustment of each calculation to separate plasma properties consistent with their alternative recycling model features is implied, via quite dissimilar patterns of reionization.

A final observation from Fig.9 refers to statistical noise within EIRENE results, alluded to above. Its presence may indeed be seen, for example, close to the target in grid rows $iy = 2$; 3 or 26; 27; 28. Compared to maximum values of the EIRENE distribution for produced ions, however, these fluctuations are down to a level of only $\sim 10^{-3}$, or a fraction of one percent. These data also involve a quite standard number of Monte Carlo trajectories, namely 2×10^4 for this outside target. While relative errors must of course be larger in some areas of strongly decreasing intrusion of neutral particle test-flights⁴, then, EIRENE source rates for ions at least could not be regarded as conspicuously less smooth than analytic functions here. Again the corresponding position concerning energy sinks has not been explored. Still there is a suggestion that noise may not be too important in standard EIRENE applications to ITER-relevant situations.

3.5 Strength of recycling

Investigations above demonstrate sensitivity of both ultimate plasma results, and “B2” numerical performance approaching them, to details of their underlying treatment of recycling source terms, even when boundary conditions do not change. Source variations considered between cases involving distinct “minimal”, Hotston or EIRENE models, however, are rather substantial, particularly regarding ion energy sinks^{2,3,4}. A much more subtle contrast is implied by instances using the same recycling approximation, as well as boundary conditions, in which only the relative *strength* of derived terms is incremented. For either “minimal” or Hotston analytic models, such a scan is very readily achieved just through alteration of a single parameter, viz ion reflection coefficient of both targets $\mathcal{R}_{IN} = \mathcal{R}_{OUT} = \mathcal{R}$.

$$\mathcal{R} = 0.99$$

Continuation from solution H_I^{zs} is shown in Fig.11, retaining Hotston recycling plus

a time-step size of 10^{-5} s, but substituting pedestal temperature boundary conditions on the perimeter and reducing ion reflection at both targets to $\mathcal{R} = 0.99$. Good convergence once more, to state H_{II}^{tp} , is apparent. A switch is then made to “minimal” sources, keeping $\mathcal{R} = 0.99$ but decreasing time-steps to 2×10^{-6} s. At least two spontaneous excursions in declining residuals, reminiscent of that in Fig.8, are exhibited, before exponential convergence to solution M_I^{tp} is eventually recovered, although at a slower rate versus cumulative iteration time.

Both portions of Fig.11 thus reproduce successful relaxation comparable to their respective earlier counterparts at higher recycling, Figs.2&8.

$\mathcal{R} = 0.98$

An opposing, more complicated response to only slightly modified sources is, though, also possible. From plasma M_I^{zs} , a well-converged, “minimal” model solution may easily be established at $\mathcal{R}_{IN} = 0.997$; $\mathcal{R}_{OUT} = 0.9985$, with temperature pedestal boundary conditions introduced on the perimeter. Continuation from this latter state is presented in Fig.12, still adopting “minimal” sources and a time-step of 4×10^{-6} s, but now attenuating target reflection coefficients to $\mathcal{R} = 0.98$.

A brief, rather chaotic phase of major amendment is seen to be followed by steady decline of residuals, then a sudden excursion of pronounced proportions which nevertheless appears completely to die away, when a highly regular, oscillatory condition instantaneously begins. The frequency, amplitude and even waveform of these oscillations are almost invariant in each equation residual, suggesting numerically cyclic iterations are being executed, and which consequently could be prolonged indefinitely.

Near-perfect oscillations as in Fig.12 might initially recall a qualitatively similar outcome of too large a time-step size, as described in ref.5 and illustrated previously for EIRENE recycling sources in Fig.5. It was already noted in §3.3 that some critical magnitude above which proper convergence of residuals can no longer be achieved⁵ may be difficult to estimate in any given situation. Yet why it should diminish between cases identical except for target reflection factors of $\mathcal{R} = 0.99$ (Fig.11) and $\mathcal{R} = 0.98$ would seem particularly obscure. A more specific test of dependence on time-steps is conducted in Fig.13, where the calculation of Fig.12 is repeated except for a limitation of their size to 10^{-6} s over the final indicated segment. Residuals plainly retrace almost exactly similar curves against cumulative iteration time, in particular with a sudden transient after the same elapsed interval and of the same duration, plus abrupt commencement of analogous oscillations with equal period ($\approx 6 \times 10^{-3}$ s $\gg$ time-step size). In other words, a unique evolution leading to a quite specific cyclic condition is precisely replicated, despite reversion to four times smaller time-steps. Under these circumstances, it is improbable that discovered oscillations could be associated just with deficiencies in time-discretization, such as found in ref.5.

Further to global measures of residuals of each plasma balance equation in Figs.12&13, extra insight into this oscillatory status may be sought by referring also to their local structure. Representations over grid indices ix, iy for the whole computational space (AFF'A')

are given in Fig.14, at the end-point of that calculation in Fig.13. While ion energy residuals appear relatively dispersed, electron energy and ion density quantities obviously are intensely concentrated around a single location. In fact, each points to a dominant, localized fluctuation of wavelength equal to the lowest resolvable by a discrete mesh, and exactly out of phase with each other. That is, maximum and minimum residual values occur in adjacent grid cells, respectively $ix = 40, iy = 22$ and $ix = 41, iy = 22$ for electron energy; $ix = 41, iy = 22$ and $ix = 40, iy = 22$ for ion density. Whether these fluctuations vary always at this one position, either up and down in magnitude or back and forth between plasma equations, through global oscillations followed in Figs.12&13 is not, of course, revealed. Note here they are disposed in a region likely to have very strongly attenuating, or minute, recycling source terms emanating from the outside target surface (cf Fig.10).

A number of other questions are prompted by preceding tests, foremost being one of their particularity, and some possible inadequacy associated with *spatial* discretization. Specificity of an oscillatory tendency to "minimal" approximation of recycling is confirmed in Fig.15, where the corresponding calculation substituting Hotston treatment is first portrayed. Starting once again from plasma H_I^s , perimeter boundary conditions for energy equations are set to temperature pedestals, time-steps of 10^{-6} s are retained, and a Hotston model with target reflection coefficients of $\mathcal{R} = 0.98$ imposed. Excellent convergence is obtained, yielding state H_{III}^{tp} , with no degradation of monotonicity other than a minor, isolated bump around ~ 0.05 s.

Switching back then to "minimal" sources and time-steps of 2×10^{-6} s as continued from H_{III}^{tp} in Fig.15, however, regular oscillations can be seen quickly to reappear. In effect a trial is constructed of repeating the "minimal" case in Figs.12&13, but proceeding from a different starting plasma, and it is clear that emergence of oscillations is strongly affected. Firstly, their onset is not precipitate as in Figs.12&13, but now gradual, while their period is roughly doubled (≈ 0.012 s $\gg$ time-step). On the other hand, their waveform qualitatively is strikingly similar. Turning to local distributions of residuals in Fig.16, another qualitative resemblance is visible, with one localized, mesh-wavelength fluctuation exactly out of phase in electron energy and ion density functions – but now in a completely distinct pair of cells $ix = 10, iy = 22$; $ix = 9, iy = 22$. These conversely imply an edge of inside target recycling sources.

Movement of residual fluctuations from one part of the computational mesh to another via alteration of starting conditions suggests that they may not arise simply due to insufficient spatial discretization, at least in any individual zone. One last check of their character is a conjecture perhaps to damp them out numerically by increased under-relaxation, available through factors applied to correction equations^{1,2} actually solved iteratively for each plasma balance relation, as outlined in §2. Ordinarily these parameters are fixed at $\frac{1}{2}$, and on the sole occasion plotted in Fig.17 they are reduced to 0.1, in conjunction with a time-step of 4×10^{-6} s, over the final labelled segment of an otherwise complete repetition of that "minimal" case in Fig.15. A small discontinuity in residuals on changing these numbers is as expected, while recurrence still of the former oscillatory pattern is subsequently clear. Examination of local distributions confirms also development of the same electron energy and density residual fluctuations in previous

inside divertor cells. Hence an identical evolution is being recovered, despite enhanced under-relaxation – although consequentially more slowly versus cumulative iteration time. This point re-emphasizes the importance cited in §2 of distinguishing between BRAAMS iteration “time”^{1,2} and real time of physical effects, when under-relaxation is employed.

Recapitulating, then, “B2” instances with “minimal” source terms at target reflections of $\mathcal{R} = 0.98$ are found to yield persistent, regular oscillations having a certain qualitative basis, namely extremely localized in electron energy and density equations, and which are maintained against variations in :-

- time-step size, to smaller values,
- plasma starting condition,
- under-relaxation of iterations, to greater degree.

On the other hand, oscillations are wholly absent if Hotston recycling replaces “minimal” description. They even disappear for the latter at a marginally higher target reflection of $\mathcal{R} = 0.99$.

Such characteristics are not suggestive of a simple numerical origin; rather that some mild mode of oscillation is defined by the complete system of “B2” difference equations^{1,2} plus “minimal” representation of recycling sources, with a growth rate which is strongly dependent (perhaps zero) on relative strength (through $\mathcal{R}$) of these latter terms. Whether this mode might also have any physical relevance is itself determined by plausibility of the specified set of model equations. Our immediate interest is just that by an alteration only of *source terms*, either qualitatively between Hotston and “minimal” analytic approximations, or modestly between “minimal” instances at $\mathcal{R} = 0.99$; $\mathcal{R} = 0.98$, BRAAMS relaxation behaviour can be markedly affected, exhibiting lastly a convergence failure of a non-numerical type. We reiterate that a revision of source terms is again applied in advancing from Hotston estimation to EIRENE.

A final incidental point in Figs.15&17 prior to interference of oscillations, and also before in Fig.11, is that each plot provides a further example of “B2” relaxation following perturbation of an already well-converged state. Here a disturbance is effected by switching from Hotston to “minimal” recycling models. As discussed formerly in §3.2, there is still an initial phase of very rapid readjustment, followed in Fig.11 at least by a resumption of slower exponential decline of residuals, identifiable potentially as its asymptotic form. Further endorsement is so given to a possible generic nature of this “B2” response for perturbed solutions.

$\mathcal{R} = 0.95$

To conclude exploration of impact of source strengths, results are shown in Fig.18 for a case incorporating perimeter temperature pedestals for energy equations, and Hotston recycling from targets with ion reflection coefficients of $\mathcal{R} = 0.95$. Time-steps are again 10^{-5} s. Once more there is good convergence, ending at plasma H_V^{tp} .

A matching calculation is depicted in Fig.19 retaining temperature pedestal boundary conditions for energy equations on the perimeter, with target reflections $\mathcal{R} = 0.95$, but substituting "minimal" source treatment and time-steps of 4×10^{-6} s. Solution M_I^{zs} is taken as a starting condition (time 0). After a noisy preliminary stage, now another, strange type of convergence failure is manifested; while ion density and electron energy residuals decay uniformly to very small magnitudes, ion energy values become decoupled, fluctuating extremely rapidly and with growing amplitude about some almost constant level. The same pattern is very faithfully repeated in Fig.20, where this "minimal" calculation is duplicated completely except for beginning from an entirely different starting plasma.

Whatever might underlie this curious behaviour, it is clear from Figs.18&19 that it must yet be associated with details of source terms. However, respective performances found between Hotston and "minimal" analytic models at $\mathcal{R} = 0.95$, and also above at $\mathcal{R} = 0.98$, might be inferred to indicate difficulties arise merely for "minimal" sources, presumably due to some complex repercussion of their comparatively primitive² structure. In progressing from Hotston to EIRENE, therefore, would related effects be absent?

Although a complete answer cannot be given, certain relevance is perhaps contained in a second counterpart of that "minimal" case in Figs.19&20. All conditions are preserved, notably $\mathcal{R} = 0.95$ and time-steps of 4×10^{-6} s, but a modification to a "1-D minimal" recycling is introduced, namely all motion of its implicit neutral particles across magnetic surfaces is *exactly* excluded. Every ion impinging from a particular magnetic flux tube (grid row *iy*) onto a target, and being recycled, can in other words interact and be reionized only within that *same* flux tube (grid row *iy*). A most beneficial outcome is displayed in Fig.21, since former pathological behaviour now is totally eliminated in favour of nominal convergence. In fact, insertion of a "1-D minimal" source model into the previous instance at $\mathcal{R} = 0.98$ also abolishes its ultimate oscillations, recovering instead uniformly decreasing residuals.

These purely formal tests serve to suggest that non-convergent evolution of "minimal" recycling calculations at $\mathcal{R} = 0.95$ and $\mathcal{R} = 0.98$ is connected with intrinsic redistribution of neutral particles across magnetic surfaces. It may be recalled from §3.4 that such a process specifically is reduced within the Hotston approximation (although still is not entirely eliminated) – but certainly is present in more realistic EIRENE description. Thus complicated features elicited with "minimal" approximation might indeed have broader significance. In any event, the key point established is that changes only in aspects of "B2" source terms clearly can profoundly alter its iterative development, potentially admitting new, unexpected modes of behaviour into the computational system of combined plasma transport plus recycling.

4. Linkage with EIRENE

4.1 Limit of convergence

Attention is now turned to specific consideration of convergence issues in BRAAMS “B2” calculations exploiting EIRENE resolution of neutral particle recycling sources. Foregoing results argue both for susceptibility of “B2” relaxation in general to details of source representations, and for possible separation of its progress during successful convergence into two phases: an initial stage of fast, major adjustment, followed by slower, asymptotic achievement of exponentially small residuals, or balance errors⁵. This latter convergence characteristic seems plainest at least for reaction to disturbance of an already well-converged state. An important possibility is that all significant adaptation of plasma properties to imposed boundary conditions could occur through-out the *preliminary* phase of rapid change, with only fine modifications being computed subsequently.

Returning to that case employing EIRENE description of recycling sources, the concluding cycles of which are shown in Fig.3, we broach again a concordant picture of repeated good convergence through each set of “short” cycles, with a recurrent perturbation at each intervening full Monte Carlo call. Recall that time-steps already appear small enough to avoid arrested relaxation of the type identified in ref.5. Still further weight is lent by extracting local ion balance errors, as defined in (1). For plasma E_{IV}^{zs} after its second set of 5000 “short” cycles in Fig.3, the greatest magnitude anywhere within outside divertor branch DFF'D' is just $|\epsilon_{\text{cellOUT}}|_{\text{max}} = 5.63 \times 10^{-4}$, according with a very high degree of consistency.

We reiterate use here with EIRENE of a distinct method of particle pumping, explained in §2, namely an albedo less than unity for neutral particles impinging on a position of an outside lower duct entrance. While this albedo is set in correspondence with a definite operating speed of some pump design, it obviously is not easy to relate to alternative target reflectivities for ions $\mathcal{R}$ adopted by Hotston and “minimal” recycling models. Derived conductance of neutral particles across the whole divertor plasma is, for instance, a dominant factor. However, if state E_{IV}^{zs} is indeed assumed to be steady, then from its flux amplification at the outside target $\mathcal{F}_{\text{OUT}} \equiv \Gamma_{\text{TOUT}}/\Gamma_{\text{SOUTHOUT}}$, which may be evaluated directly, an effective target reflection may be inferred according to $\hat{\mathcal{R}}_{\text{OUT}} = (\mathcal{F}_{\text{OUT}} - 1)/\mathcal{F}_{\text{OUT}}$. Inserting obtained $\mathcal{F}_{\text{OUT}} = 287.81$ yields $\hat{\mathcal{R}}_{\text{OUT}} = 0.9965$. This figure hence is also within the regime of good numerical performance for both analytic source treatments above, significantly higher than a level under which inhibition of convergence was encountered for more distributed “minimal” deposition of neutral particles.

Although all instances described have been exclusively for a typical ITER problem, it may be added that entirely equivalent performance of “B2”/EIRENE cycles has been found in a variety of other, quite different divertor plasma situations, ie smaller configurations, lower densities and power through-puts, lower recycling regimes, etc. These independent studies will be documented elsewhere, but they too reinforce evident generality of that pattern of repetitive “short” cycle relaxations plus full Monte Carlo deviations under scrutiny.

The clear question remaining is why each full EIRENE call should exert an almost constant perturbation to conditions determined after each group of “short” cycles. Even after a large number of “B2”/full EIRENE cycles these disturbances do not diminish, so that recovery of residuals during a next “short” sequence tends itself to approach a constant lower bound, and effectively no further evolution of a solution is produced. In this situation, it might therefore be deduced that convergence to the *technical* limit of a particular implementation had been achieved, if :-

- a) characteristically two-stage reduction of residuals always to a similar level through each “short” series signifies their good degree of convergence, and
- b) departures at each full Monte Carlo intervention arise for essentially *technical* reasons.

We consider a technical basis of “short”/full EIRENE cycle incompatibilities, and their implications, in subsequent sections.

4.2 Statistics

One inherently variable component in full Monte Carlo sources is statistical noise, so that some discrepancies between any pair of full EIRENE calls might seem inevitable. It was ascertained in §3.4, however, that statistical fluctuations already appear very small in relative magnitude for a moderate number of sample trajectories ($\sim 2 \times 10^4$). Moreover, a particular technique of “correlation sampling”¹³ is employed which reduces their variability still further, as follows.

“Random” number generators employed in Monte Carlo codes are in reality perfectly deterministic, in that from any single member in a series all its succeeding members can be reproduced exactly, a property conventionally denoted “pseudo-randomness”. There is a capability⁴ deliberately to exploit it within EIRENE, though, by using in consecutive calculations the same set of initial “seed” numbers for each “random” sequence pertaining to a neutral particle test-flight. In other words, identical progressions of numbers will be produced for each trajectory, so that if the background plasma and its consequent target launching distribution(s) do not change between two applications, then EIRENE will recompute the same interactions and sources *exactly*^{4,6,13}. More practically, when small changes in plasma details are still occurring, the effect will be to induce a strong *positive correlation*^{4,6} between successive EIRENE results, and in a much more robust manner than is achievable with only one fixed “seed” number for a whole Monte Carlo run. Simultaneously, as mentioned above, statistical structure becomes much less unsteady.

A highly favourable impact of positive correlation for ITER divertor simulations is illustrated in Fig.22. This traces development of normalized errors in ion number and total energy balances over outside divertor sector DFF'D', referred to in §3.3 previously. Respective measures $\epsilon_{n_{OUT}}$; $\epsilon_{Q_{OUT}}$ are defined by⁵ :-

$$\epsilon_{n_{OUT}} \equiv \frac{1}{\int_{S_{TOUT}} \Gamma \cdot dS} \left(\int_{S_{SOUTHOUT}} \Gamma \cdot dS - \int_{S_{TOUT}} \Gamma \cdot dS + \int_{V_{OUT}} S_n dV \right) ;$$

$$\epsilon_{Q_{OUT}} \equiv \frac{1}{Q_{SOUTH_{OUT}}^{e+i}} \left(Q_{SOUTH_{OUT}}^{e+i} - Q_{TOUT}^{e+i} + \int_{V_{OUT}} S_Q^{e+i} dV \right),$$

where S are appropriate surfaces of integration, Q (W) are total energy fluxes, S_Q ($\text{W}\cdot\text{m}^{-3}$) are energy volumetric source rates, and superscripts $e+i$ signify summation of electron and ion components. Note that since both expressions neglect fluxes possibly flowing to outermost (grid “North”) and private region boundaries, they may be expected to become small but not necessarily zero close to steady states. Global quantity $\epsilon_{n_{OUT}}$ also has to be less sensitive than former local error $|\epsilon_{\text{cell}_{OUT}}|_{\text{max}}$ from (1), owing to its normalization by a much greater denominator.

The first four cycles in Fig.22 will be recognized as a rehearsal of Fig.6, leading to plasmas E_I^{zs} ; E_{II}^{zs} . Recall that time-steps involved are excessively large, obstructing convergence (cf Fig.5), despite marginally decreasing (if noisy) trends of $|\epsilon_{n_{OUT}}|$; $|\epsilon_{Q_{OUT}}|$. One underlying factor responsible is their incorporation of positive correlation, as revealed by continued cycles with a reduced time-step of 4×10^{-6} s but *no* correlation of full EIRENE interventions. While strong fluctuations in balance errors disappear immediately on recourse to smaller, legitimate time-steps, improper increasing trends then emerge without assistance from positive correlation. Remaining large spikes in $|\epsilon_{Q_{OUT}}|$ arise simply when errors alternate in sign.

A final corresponding picture is plotted in Fig.23, depicting $|\epsilon_{n_{OUT}}|$; $|\epsilon_{Q_{OUT}}|$ for those improved cycles ending in states E_{III}^{zs} ; E_{IV}^{zs} ; E_V^{zs} first introduced in Fig.3. We reiterate valid time-steps are taken, and positive correlation is included as well. Smooth curves around low magnitudes, with $|\epsilon_{n_{OUT}}|$ in particular dropping uniformly through the sequence, are a last corroboration of their proposed status of effectively being converged.

Use of standard samples of Monte Carlo histories together with positive correlation therefore seems to limit the influence of statistical fluctuations contained in full EIRENE calls. Other contributions are indicated to discontinuities they incur in “B2” residuals.

4.3 Inequivalences of “short” & full EIRENE calls

Given restricted impression of statistics on EIRENE recycling sources, a naïve idealization of linked execution would be just to request a complete Monte Carlo evaluation at every BRAAMS internal iteration^{1,2}. In this manner, its extensive treatment would stay always precisely in synchrony with evolving plasma properties, exactly as accomplished with simpler Hotston and “minimal” analytic models. Convergence directly towards consistency of plasma and detailed neutral particle descriptions might similarly be contemplated. Such an approach is not (yet) practicable, however, owing to excessive computation times which would be demanded.

For pragmatic reasons, it is therefore obligatory greatly to reduce the frequency of full EIRENE calls, and between to interpose lesser, so-called “short” cycles⁶ at each “B2” internal iteration. During these, source terms are *approximately* up-dated according to simultaneous plasma values. An account of this procedure has been given before in ref.6, but the crucial logic of short-cycle revisions may be exemplified by reference to one specific

component in ion energy source rates, namely that volumetric power deriving from atomic charge-exchange reactions ζ_i^{cx} ($\text{W}\cdot\text{m}^{-3}$).

A kinetic relation for ζ_i^{cx} at some position and instant may be written^{4,6} :-

$$\zeta_i^{\text{cx}} = n_i n_o \int d\mathbf{v}_o f_o(\mathbf{v}_o) \left\{ \frac{1}{2} m_o v_o^2 \langle \sigma^{\text{cx}} | \mathbf{v}_o - \mathbf{v}_i | \rangle - \langle \sigma^{\text{cx}} | \mathbf{v}_o - \mathbf{v}_i | \frac{1}{2} m_i v_i^2 \rangle \right\} \quad (2)$$

where subscripts o ; i denote respectively neutral atom and ion quantities, f_o is the atomic distribution function, normalized such that $\int d\mathbf{v}_o f_o = 1$, σ^{cx} (m^2) is a two-body cross-section, and angled brackets $\langle \rangle$ imply integration over the normalized ion distribution function, ie $\langle a \rangle \equiv \int d\mathbf{v}_i f_i(\mathbf{v}_i) a$. A common approximation⁴ is then to estimate this by a drifting Maxwellian, in which case bracketed terms become functions only of $\mathbf{v}_o$; T_i and $\langle \mathbf{v}_i \rangle \equiv \mathbf{v}_i$.

For convenience, we adopt notations for atomic integrals :-

$$\begin{aligned} \mathcal{I}_I &\equiv n_o \int d\mathbf{v}_o f_o(\mathbf{v}_o) \frac{1}{2} m_o v_o^2 \langle \sigma^{\text{cx}} | \mathbf{v}_o - \mathbf{v}_i | \rangle \quad (\text{W}) ; \\ \mathcal{I}_{II} &\equiv n_o \int d\mathbf{v}_o f_o(\mathbf{v}_o) \langle \sigma^{\text{cx}} | \mathbf{v}_o - \mathbf{v}_i | \frac{1}{2} m_i v_i^2 \rangle \quad (\text{W}) ; \\ \mathcal{I}_{III} &\equiv n_o \int d\mathbf{v}_o f_o(\mathbf{v}_o) \langle \sigma^{\text{cx}} | \mathbf{v}_o - \mathbf{v}_i | \rangle \quad (\text{s}^{-1}) , \end{aligned}$$

so that (2) becomes $\zeta_i^{\text{cx}} = n_i [\mathcal{I}_I - \mathcal{I}_{II}]$, and $\mathcal{I}_{II} \approx \left(\frac{3}{2} T_i + \frac{1}{2} m_i v_i^2 \right) \mathcal{I}_{III}$ with small error in a range where typically⁴ $\sigma^{\text{cx}} \sim \frac{1}{|\mathbf{v}_o - \mathbf{v}_i|}$.

Now full EIRENE applications accurately compute moments $\mathcal{I}_I$; $\mathcal{I}_{II}$; $\mathcal{I}_{III}$ etc of neutral particle distribution f_o , and so effects like ζ_i^{cx} , by Monte Carlo synthesis explicitly of their kinetic integrals. During intermediate "short" cycles, these can accordingly be estimated only from their most recent, preceding full EIRENE determination, designated by superscripts $\mathcal{I}_I^{[o]}$ etc. Each rate actually required at former "short" iterations, indicated by superscripts for instance on charge-exchange power $\zeta_i^{\text{cx}[n]}$, must be suitably approximated, with some degree of *implicitness* on instantaneous plasma details.

Firstly, each component $\mathcal{I}_I$; $\mathcal{I}_{II}$; $\mathcal{I}_{III}$ etc can be seen to depend linearly on neutral particle density n_o , which itself scales linearly with originating ion flux (s^{-1}) to whatever portion of a target is being handled. That is, recycling source contributions may be accumulated from a whole target at once, or in several additive parts from smaller sub-sections treated separately. In either case, all associated such terms and dependent rates like ζ_i^{cx} are multiplied by a factor $\gamma^{[n]}$ at "short" iterations, where :-

$$n_o^{[n]} = \gamma^{[n]} n_o^{[o]} \Leftrightarrow \gamma^{[n]} = \frac{\int_{S_T} \Gamma^{[n]} \cdot d\mathbf{S}}{\int_{S_T} \Gamma^{[o]} \cdot d\mathbf{S}} .$$

A certain formula regarding ζ_i^{cx} may secondly be considered, viz :-

$$\gamma^{[n]} \left\{ \zeta_i^{\text{cx}[o]} + \left(n_i^{[n]} - n_i^{[o]} \right) \mathcal{I}_I^{[o]} - \left(\frac{3}{2} \left[n_i^{[n]} T_i^{[n]} - n_i^{[o]} T_i^{[o]} \right] + \frac{1}{2} m_i \left[n_i^{[n]} v_i^{[n]2} - n_i^{[o]} v_i^{[o]2} \right] \right) \mathcal{I}_{III}^{[o]} \right\} \quad (3)$$

$$\begin{aligned}
&= n_i^{[n]} \gamma^{[n]} \mathcal{I}_I^{[o]} - \left[n_i^{[n]} \left\{ \frac{3}{2} T_i^{[n]} + \frac{1}{2} m_i \nu_i^{[n]2} \right\} \gamma^{[n]} \mathcal{I}_{III}^{[o]} + \gamma^{[n]} n_i^{[o]} \left(\mathcal{I}_{II}^{[o]} - \left\{ \frac{3}{2} T_i^{[o]} + \frac{1}{2} m_i \nu_i^{[o]2} \right\} \mathcal{I}_{III}^{[o]} \right) \right] \\
&\equiv \tilde{\zeta}_i^{cx[n]} \sim n_i^{[n]} \mathcal{I}_I^{[n]} - n_i^{[n]} \mathcal{I}_{II}^{[n]} = \zeta_i^{cx[n]}.
\end{aligned}$$

Thus (3) adjusts atomic charge-exchange power through-out “short” cycles, attempting to represent its accommodation to momentary plasma conditions $n_i^{[n]}$; $T_i^{[n]}$; $\nu_i^{[n]}$; in this sense, its up-dating is rendered implicit. Integral $\mathcal{I}_{II}$ specifically is estimated exploiting $n_i \mathcal{I}_{II} \approx n_i (\frac{3}{2} T_i + \frac{1}{2} m_i \nu_i^2) \mathcal{I}_{III}$, and indeed it follows that marginally higher implicitness even could be derived from $\mathcal{I}_{II}^{[n]} \approx \left\{ (\frac{3}{2} T_i^{[n]} + \frac{1}{2} m_i \nu_i^{[n]2}) \gamma^{[n]} \mathcal{I}_{III}^{[o]} + \varepsilon_{II}^{[n]} \right\}$ by presuming expressly a decrement $\varepsilon_{II}^{[n]} \approx \gamma^{[n]} \varepsilon_{II}^{[o]} = \gamma^{[n]} \left\{ \mathcal{I}_{II}^{[o]} - (\frac{3}{2} T_i^{[o]} + \frac{1}{2} m_i \nu_i^{[o]2}) \mathcal{I}_{III}^{[o]} \right\}$. A slightly modified formula would result :-

$$\begin{aligned}
\zeta_i^{cx[n]} &\sim \tilde{\zeta}_i^{cx[n]} \\
&\equiv n_i^{[n]} \gamma^{[n]} \left\{ \mathcal{I}_I^{[o]} - \left[\left(\frac{3}{2} T_i^{[n]} + \frac{1}{2} m_i \nu_i^{[n]2} \right) \mathcal{I}_{III}^{[o]} + \left\{ \mathcal{I}_{II}^{[o]} - \left(\frac{3}{2} T_i^{[o]} + \frac{1}{2} m_i \nu_i^{[o]2} \right) \mathcal{I}_{III}^{[o]} \right\} \right] \right\} \\
&= n_i^{[n]} \gamma^{[n]} \left\{ \frac{\zeta_i^{cx[o]}}{n_i^{[o]}} - \left(\frac{3}{2} [T_i^{[n]} - T_i^{[o]}] + \frac{1}{2} m_i [\nu_i^{[n]2} - \nu_i^{[o]2}] \right) \mathcal{I}_{III}^{[o]} \right\},
\end{aligned}$$

in which then, unlike in (3), assumed decrement $\gamma^{[n]} \varepsilon_{II}^{[o]}$ also would scale with current ion density $n_i^{[n]}$.

The importance of implicitness within “short” iterations is exposed by recalling that contrast in behaviour disclosed between “B2”/EIRENE cycles in Figs.3&7. The sole difference between the former successful and latter abortive “short” sequences, as referred to in §3.3 above, is a marginally more implicit approximation of charge-exchange power density ζ_i^{cx} in Fig.3. While this incorporates $\tilde{\zeta}_i^{cx[n]} \sim \zeta_i^{cx[n]}$ as in (3), in Fig.7 its underlying estimate omitted adjustment also with the current ion *temperature*, ie equivalent to reverting $T_i^{[n]}$ just to $T_i^{[o]}$ in (3). Even such a minor improvement in assimilating developing plasma values is hence enough to effect stable cycles.

It is clear that in a limit of perfect convergence when $n_i^{[n]} \rightarrow n_i^{[o]}$; $T_i^{[n]} \rightarrow T_i^{[o]}$; $\nu_i^{[n]} \rightarrow \nu_i^{[o]}$; $\Leftarrow \gamma^{[n]} \rightarrow 1$ etc, intermediate estimates like (3) would approach their full Monte Carlo terms, eg $\tilde{\zeta}_i^{cx[n]} \rightarrow \zeta_i^{cx[o]} \rightarrow \zeta_i^{cx[n]}$, and “short” cycles would become equivalent asymptotically to full evaluations. Significantly, however, “short” iterations will otherwise always be *distinct*; that is, in *practice*, they will remain *inequivalent* to full Monte Carlo contributions.

The impact may then be considered at each complete EIRENE invocation late in a converging series of outer cycles with “B2”. Whilst representations at the end of its immediately preceding “short” sequence (furnishing next quantities $n_i^{[o]}$; $T_i^{[o]}$ etc) are not totally consistent, full EIRENE will return new sources which are somewhat different from their last “short” estimates. As discussed previously, these necessarily connote *modified* consistent plasma conditions. On a first subsequent internal iteration of “B2” in a next “short” episode, therefore, these altered values will be pursued, and succeeding first imposition of

source approximations such as (3) will inevitably include non-zero departures $n_i^{[1]} \neq n_i^{[0]}$; $T_i^{[1]} \neq T_i^{[0]}$ etc. Short-cycle source approximations will thus act as a *different* model, so that (stable) continuing iterations will once more tend to converge to other plasma properties consistent with distinct terms, eg $\tilde{\zeta}_i^{cx[n]} \neq \zeta_i^{cx[n]}$ ($\{n_i^{[n]} - n_i^{[0]}\} \rightarrow \text{constant} \neq 0$; $\{T_i^{[n]} - T_i^{[0]}\} \rightarrow \text{constant} \neq 0$ etc). This process could consequently repeat indefinitely, with eventually the same end and start of cycle states always being recovered. A roughly constant, recurrent perturbation between “short” and full EIRENE calculations will result, directly related itself to inequivalences between their respective approximate and comprehensive source descriptions.

In effect, the short-cycle source estimations serve as a further type of analytic model, with disturbances of residuals occurring between them and full Monte Carlo executions just as was seen more severely when a switch was made from Hotston to “minimal” recycling in Figs.11&15. Local particle balance errors ϵ_{cell} as defined in (1), for instance, will be reduced to small values in accordance with “short” production rates $\tilde{S}_n$, but these balances will tend to be destroyed again at the next determination of correct EIRENE sources S_n . Once all other initial discrepancies have been relaxed away, additional cycles will come to be dominated by their alternating inequivalences, and a pattern of persistent jumps and recoveries in “B2” residuals as first illustrated in Fig.3 will tend to be established. The foregoing argument suggests that such a pattern is unavoidable for any short-cycle scaling treatment not essentially identical to full Monte Carlo applications. Moreover, it will approach some lower level which will only decline unacceptably slowly, or potentially not at all, so that further convergence will not be possible by prolonging the cycling. It is important to recall also that solutions are required which are consistent with the most physical, *full* EIRENE recycling, incorporated only at complete Monte Carlo calculations. There may be little benefit either, then, in increasing numbers of intermediate “short” cycles, eg by widening the tolerances⁶ for global alterations of last full values, or raising the ceiling number⁶ of “short” iterations (cf §3.1).

To summarize, in a stable series of “B2”/EIRENE cycles, residuals are liable ultimately to settle to a base of sustained perturbations of roughly constant amplitude at each full EIRENE intervention after a set of “short” iterations. These disturbances are attributable, and in proportion, to :-

- inequivalences between sources as determined by "short" scaling approximations and full Monte Carlo calculations. These both influence stability of the cycles and govern their final level of convergence, ie concluding magnitudes of residuals. Greater equivalence between treatments should promote stability and reduce larger values to which residuals are returned at full Monte Carlo steps.

For a given short-cycle formulation, ie a particular degree of inequivalence with complete EIRENE description, the limiting perturbation corresponding to full-cycle reintroduction of the latter sources will effectively be fixed, and hence so will that level to which residuals tend to be restored. When unvarying perturbations are encountered at each cycle, therefore, no advantage may derive from greater numbers of intermediate "short" iterations; they could affect only an incidental tendency to small, pre-disturbance values (cf Fig.3). "Short" stages might then be abbreviated without loss of detail in solutions.

- to an extent, perturbative levels of residuals retrieved at each full EIRENE cycle are affected also by the number of neutral particle histories they include. In other words, statistics of Monte Carlo computations

of recycling sources do indeed add a second component into the discontinuities, although with positive correlation the dependence may be weak, as previously noted. A decrease of noise, and so limiting residuals, at most with the square root of numerical sample size⁴ might be expected, typifying a law of large numbers. For moderate numbers of trajectories, large further increases in Monte Carlo calculations could be necessary to make an appreciable improvement in convergence levels.

4.4 Improvements to linkage

Various possibilities follow from the foregoing discussion for improving technically the linkage of "B2" and EIRENE transport models. In this regard, three aspects of such cycles should be recognized :-

- stability,
- rate of convergence,
- level of convergence.

We itemize certain propositions potentially impinging on each of these characteristics.

- i) Primarily, it has been implied above that a better level of convergence should proceed from greater equivalence of short-cycle source approximations to full Monte Carlo terms. Higher implicitness of "short" expressions, eg (3), is one prominent means to pursue this, and which seems simultaneously to enhance stability of associated iterations (cf Figs.3&7).

In practice, charge-exchange ion energy loss ζ_i^{cx} as in (2) is generally a critical component in behaviour of linked cycles. Commonly it describes a small difference of two large factors (cf (2)), so being susceptible numerically to relatively large fluctuations in values. Any extension of implicitness in its short-cycle scaling, then, could be especially beneficial. In fact, a fully implicit formula can be defined, at the expense of evaluating in and carrying from EIRENE certain extra neutral particle moments, and could be an amendment to implement next.

- ii) Also demonstrated was the favourable effect of positive correlation between successive Monte Carlo executions, not only in promoting stability (cf Figs.22&23), but also possibly accelerating convergence. Stronger impositions could again be sought.

Complete strategies for accentuating positive correlation are well-established in the formalism of Monte Carlo propagation problems. In iterative neutron dynamics in particular, techniques have been devised of resampling from early generations of numerical distribution functions, with adjustments through succeeding iterations being accommodated in analytic weighting functions. Increasing positive correlation is provided by computing weighting functions further and further

through Monte Carlo progressions of instantaneous distributions, until ultimately unit positive correlation would result from a wholly *analytic* calculation modifying weights for a fixed, complete set of sample trajectories. A preliminary analogy might be constructed in the present case, for instance, by extending existing reproduction of underlying sequences of pseudo-random numbers⁴ (cf §4.2) to resampling from invariant target launching distributions.

A second, explicit procedure may be realized by involving at each full EIRENE cycle $[\ell]$, beginning after some initial number $[k]$, not those source terms immediately so determined, eg $S_n^{[\ell]}$ etc, but instead "damped" forms :-

$$\check{S}_n^{[\ell]} \equiv \left\{ \int S_n^{[\ell]} dV \right\} \frac{\left\{ S_n^{[\ell]} / \int S_n^{[\ell]} dV \right\} + \alpha \left\{ \check{S}_n^{[\ell-1]} / \int S_n^{[\ell-1]} dV \right\}}{1 + \alpha} ; \quad (4)$$

$(\ell > k; \check{S}_n^{[k]} \equiv S_n^{[k]}) ,$

where α is some chosen under-relaxation parameter. If specifically $\alpha \equiv (\ell - k)$, viz :-

$$\check{S}_n^{[\ell]} = \left\{ \int S_n^{[\ell]} dV \right\} \frac{\left\{ S_n^{[\ell]} / \int S_n^{[\ell]} dV \right\} + (\ell - k) \left\{ \check{S}_n^{[\ell-1]} / \int S_n^{[\ell-1]} dV \right\}}{1 + \ell - k} ; \quad (\ell \geq k) , \quad (5)$$

then $\check{S}_n^{[\ell]}$ becomes simply the arithmetic mean of normalized Monte Carlo sources $\left\{ S_n^{[\ell]} / \int S_n^{[\ell]} dV \right\}$ over full cycles $(k, k+1, \dots, \ell)$. Admission of a threshold $[k]$ activates damping only after preliminary cycles spanning major relaxation of properties, and when limiting, repetitive perturbations have been achieved.

Such formulae were first suggested near the start of development of "B2"/EIRENE linkage methods¹², prospectively to smooth high-frequency statistical or numerical fluctuations over cycles. A closely related treatment has recently been investigated in an independent study¹⁴. Importantly, though, remarks in §4.2 should be recalled concerning effects of correlation sampling. Namely, positive correlation when applied tends to eliminate *statistical* noise as convergence is approached, by recovering increasingly similar sets of Monte Carlo trajectories. A weighted aggregation of samplings of some form (4) would then act chiefly to reinforce their positive correlation, although now obviously at a cost of slowing down any continuing convergence. Other *numerical* oscillations, if present, should simultaneously tend to be suppressed.

In principle, converse negative correlation could also be used in full EIRENE calls, together with an expression (4). While this option⁴ is not presently implemented within EIRENE, by emphasizing its statistical fluctuations before applying supplementary smoothing (4), it could particularly diminish statistical errors. Alternatively, fewer histories might be needed to achieve some desired level.

- iii) Another technique anticipated in early "B2"/EIRENE trials¹², and recalled in §4.3 above, could perhaps aid convergence of attendant cycling. "Short" rescaling of Monte Carlo sources, as in (3), may be performed on values computed for a whole target plate at once, or separately on several sets of functions each arising from constituent portions of a target¹². This sub-division into multiple components or "strata" per target, which has now been made available in the latest EIRENE coupling, introduces an extra degree of freedom into short-cycle treatments, possibly improving their adaptiveness, particularly with regard to *transverse* (σ_y) alterations of distributions. It relates in effect to a capability of statistical methods to be optimized with respect to any selected error term, through a suitable, legal statement.
- iv) One last recourse to seek most consistent combination of "B2" and EIRENE might be finally to adopt their *direct* union as cited in §4.3, ie to include a full EIRENE execution at every "B2" internal iteration, dispensing with "short" cycles altogether.

As noted before, this is clearly not practicable through-out a long calculation, but could eventually become viable if foregoing interpretations of convergence behaviour are correct. That is, when cycles settle to a pattern of roughly unchanging perturbations, relaxation to boundary conditions could largely have been accomplished, and mean saturation of residuals may reflect chiefly just incompatibilities between alternating "short" and Monte Carlo recycling sources. At such a stage, a relatively brief ($\sim 10^2$) series of direct "B2" plus full EIRENE iterations, with moderate numbers ($\text{few} \times 10^4$) of neutral particle test-flights per target, might be feasible. Averaging of EIRENE results, following (4), might additionally be applied. The outcome suggested would be to allow a last, modest adjustment, to a solution offering closest consistency with complete Monte Carlo description of recycling, as demanded.

4.5 Pragmatic criterion of convergence

While preceding suggestions may enhance convergence of "B2"/EIRENE cycles, it is evident that at least without successful, direct iterations as outlined in iv), some type of full plus intermediate "short" alternation will remain. Furthermore, these will retain generally some inequivalences in their respective source identifications. According to arguments presented, therefore, serial disturbances should ultimately be expected to recur between them, causing residuals to stabilize around some roughly constant mean level. We return now to our original question of whether such behaviour, as first exemplified in Fig.3, can in fact be considered as signifying satisfactory convergence⁵.

Essentially it is contended that major relaxation to boundary conditions has indeed occurred by this closing phase. Thus adjustments still proceeding may be only minor, and attributable largely to repeated accommodation of differences in source terms being exerted between "short" and full EIRENE steps. That is, establishment of ideal, prolonged exponential decays of residuals⁵ is inhibited by purely technical factors. On such a basis,

a pragmatic restatement of the former perfect definition of asymptotic convergence (cf §3.1) is thus proposed :-

- In a given "B2"/EIRENE calculation, initial substantial variations in residuals should have elapsed, plus an average decreasing trend should have been evident, evolving into cycles comprising long sequences of "short" iterations interrupted by consistent perturbations at each full EIRENE invocation. These discontinuities should become of almost constant amplitude, leading to maintenance of nearly fixed average levels of residuals.
- For purposes of confirmation, it should be specifically demonstrable that key properties of interest, eg near-strike-point plasma temperatures or transverse profiles etc, are then no longer varying significantly, except perhaps for fluctuations induced at foregoing "short" to full cycle perturbations.
- Finally, it should be testable that no significant alterations to development of residuals or local properties are exhibited when the calculation is now continued with a *reduced* "B2" time-step. A momentary shock to values of residuals may accompany an abrupt decrease in iterative time-step, but a return to the same qualitative pattern of uniform "short" to full cycle disturbances, and particularly to identical values of local quantities, should rapidly ensue. This check consequently ensures that no discrepancies are still lingering due to an excessive time-step (cf §3.3), of a type as first discussed in ref.5.

If these practical conditions are met, it is recommended that the associated "B2"/EIRENE state might actually be taken as an adequately converged solution.

5. Summary

Realistic numerical studies of tokamak divertors require comprehensive treatments of both edge plasma and recycled neutral particle transport, such as provided by combination of the respective BRAAMS "B2" and EIRENE Monte Carlo steady-state models. Earlier "B2" studies⁵ involving a simpler, analytic approximation of recycling sources had already exposed the importance of ensuring valid convergence of calculations in order to extract reliable solutions; a fundamental difficulty is that similar ideal exponential decays of residuals are not reproduced in conjunction with EIRENE (or equivalent) description.

Using a system representative of conditions expected for the ITER divertor, test calculations varying only analytic estimates of source terms in otherwise identical problems revealed an accompanying capability for radically different forms of relaxation behaviour. Merely switching between so-called Hotston³ and "minimal"² recycling models, new situations can be accessed in which residuals *oscillate* regularly and indefinitely, with no further tendency either to diminish or to grow. These oscillations are unaffected by decreasing the size of iterative time-steps, and hence are not related to numerical deficiencies associated with excessively large values of the latter, of a type disclosed in ref.5. Neither can they be abolished by greater under-relaxation or change of starting state. They can alter markedly in character even for modifications just in the strength of recycling (ie pumping) with the single "minimal" model.

Such oscillations appear to refer to highly localized fluctuations in plasma properties, which might themselves be connected with natural redistribution of neutral particle sources across magnetic surfaces. Effective suppression of these transverse motions in the Hotston model, and consequent inhibition of inward relocation of sources at long range, may for example feature in its exceptional favourability regarding stability and exponential convergence. In any event, contrasting effects in cases differing only in representations of recycling indicate that amendments in details of source terms can profoundly alter the behaviour. New modes can be admitted which are *intrinsic* to the specified complete system of plasma transport plus neutral sources. These can result in convergence failures, then, of *non-numerical* kind.

Even under circumstances of optimum convergence, typical of incorporating Hotston recycling, a characteristic evolution of residuals in two definite phases is discernible: a first interval of rapid, sometimes noisy decline, succeeded by generally slower but sustained exponential decays. A possible explanation is that principal adaptation to boundary conditions actually occurs during the initial, busy stage, with only lesser refinements of properties continuing thereafter.

Best relaxation of "B2" with EIRENE resolution of sources displays a further pattern of residuals, which qualitatively is found for a variety of scrape-off layer problems in addition to the ITER divertor. Practicable cycles of both models involve intermittent executions of full Monte Carlo integrations, with reduced, so-called "short" cycles implicitly rescaling source rates at every "B2" internal iteration between. Now after a preliminary, busy period of joint cycling, a trend eventually emerges, consisting of falling residuals through long sequences of "short" iterations, before each automatic recourse to a full

EIRENE step, upon which they are immediately returned to larger values. These perturbations become roughly constant in magnitude, so that similar series of "short" iterations and discontinuities tend to be repeated, with residuals maintaining almost uniform mean levels.

Again difficulties are not arising due to excessively large time-steps, and moreover statistical noise in Monte Carlo terms is effectively limited by use of positive correlation between estimations. Recurrent disturbances are thus probably induced by *inequivalences* in "short" and full EIRENE source treatments, leading to departures of their corresponding steady states being persistently reintroduced at alternating invocations. Numbers of Monte Carlo sample trajectories also contribute a secondary component in the mean level established. Solutions required, of course, correspond to *full* EIRENE recycling, and hence thereafter little advantage may follow from increasing numbers of "short" cycles between its perturbing applications.

On this basis, various techniques are implied which potentially might improve both stability and convergence of "B2"/EIRENE cycles. Essentially, greater consistency of "short" and full sources should be sought, for example by higher implicitness of former rescalings, while stronger positive correlation of Monte Carlo executions could also be beneficial, for instance simply by aggregation of successive samplings. Ultimately, a relatively brief series of cycles with a complete EIRENE call at every "B2" internal iteration could be attempted, for total model synthesis.

In general, however, restrictive perturbations might be expected to remain in a scheme of Monte Carlo and "short" estimated sources alternation. Exponential convergence of residuals, therefore, seems to be prevented by purely *technical* constraints. A pragmatic restatement of a criterion of convergence is suggested, namely that a "B2"/EIRENE state might be accepted as an adequately relaxed solution if (a) repetitive, fixed perturbations effecting mean saturation of residuals have been achieved, and (b) there is confirmation from local properties not changing significantly for continuation with a *reduced* iterative time-step. In other words, present linked calculations should be leading to correct results. While exponential decreases of residuals are unequivocally a sufficient signature of valid convergence to a steady state, they may not strictly be necessary in the presence of technical impediments.

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Table 2. “B2” states with given recycling approximations

State	time-step (10^{-6} s)	Reflect. $\mathcal{R}_{\text{OUT}}$	Flux amp. $\mathcal{F}_{\text{OUT}}$	ion bal. error $ \epsilon_{\text{cellOUT}} _{\text{max}}$
$\text{H}_\text{I}^{\text{zs}}$	10	0.9985	667.10	2.03×10^{-5}
$\text{H}_\text{I}^{\text{tp}}$	10	0.9985		
$\text{H}_\text{II}^{\text{tp}}$	10	0.99	100.42	
$\text{H}_\text{III}^{\text{tp}}$	10	0.98	49.995	
$\text{H}_\text{IV}^{\text{tp}}$	10	0.95	19.981	

$\text{M}_\text{I}^{\text{zs}}$	4	0.9985	787.15	$290. \times 10^{-5}$
$\text{M}_\text{I}^{\text{tp}}$	2	0.99		

		$\hat{\mathcal{R}}_{\text{OUT}}$		
$\text{E}_\text{IV}^{\text{zs}}$	4	0.9965	287.81	56.3×10^{-5}
$\text{E}_\text{I}^{\text{zs}} ; \text{E}_\text{II}^{\text{zs}}$	40	<i>oscillatory convergence failure</i>		

Fig.1 ITER CDA Double-null (lower half)
discrete geometry & computational map

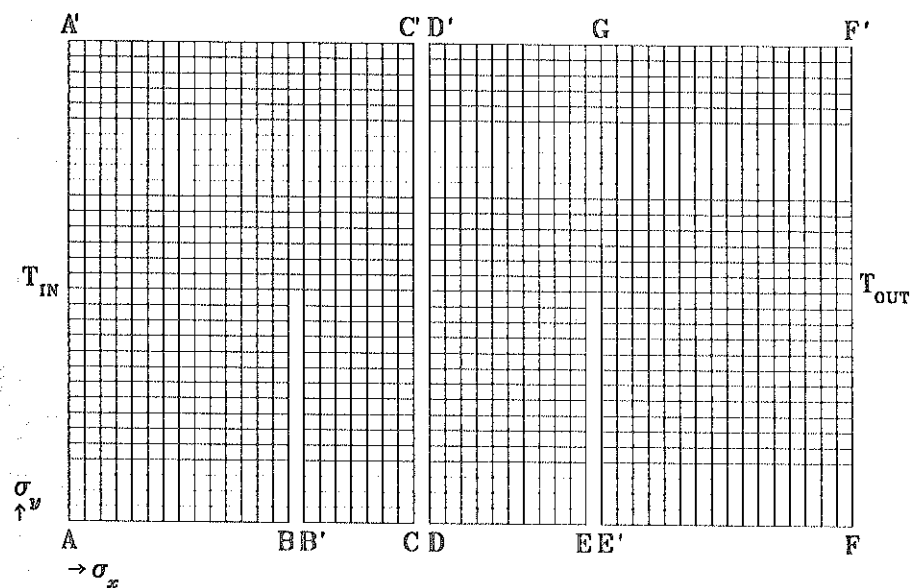
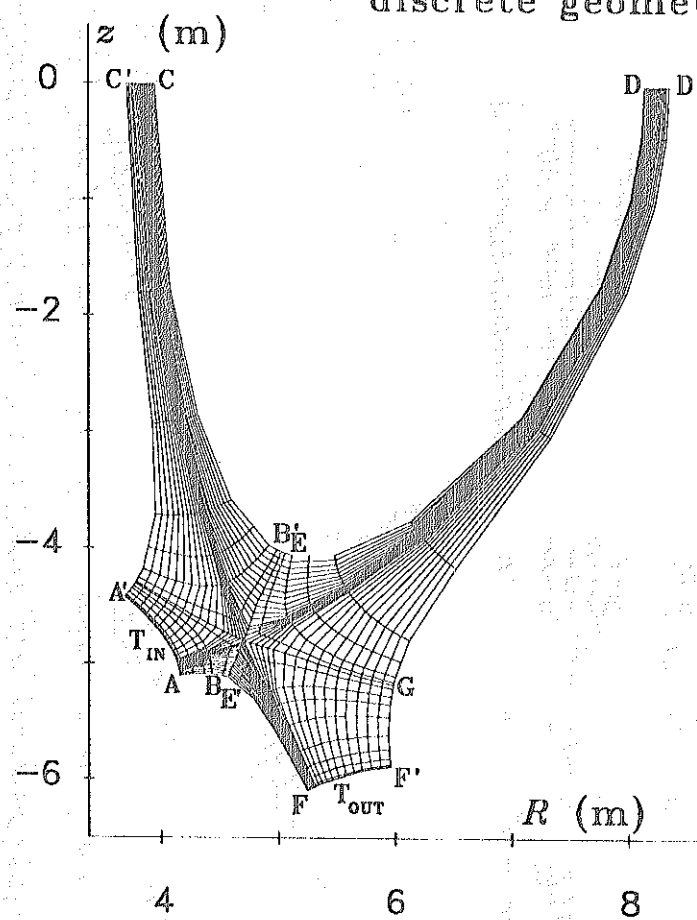


Fig.2 Evolution of "B2" residuals – Hotston recycling

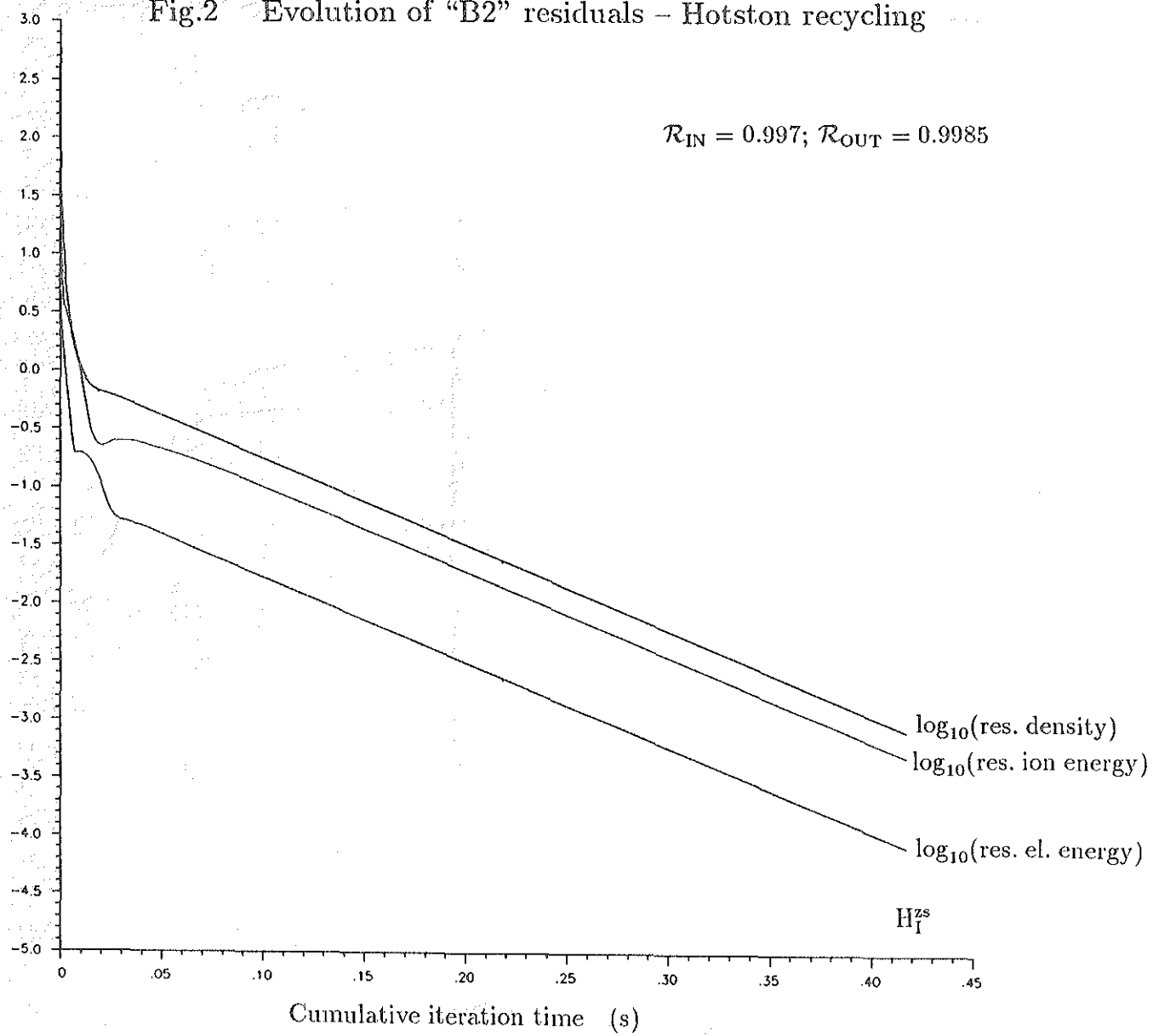


Fig.3 Evolution of "B2"+EIRENE cycles
(6×10^4 test-flights each Monte Carlo call)

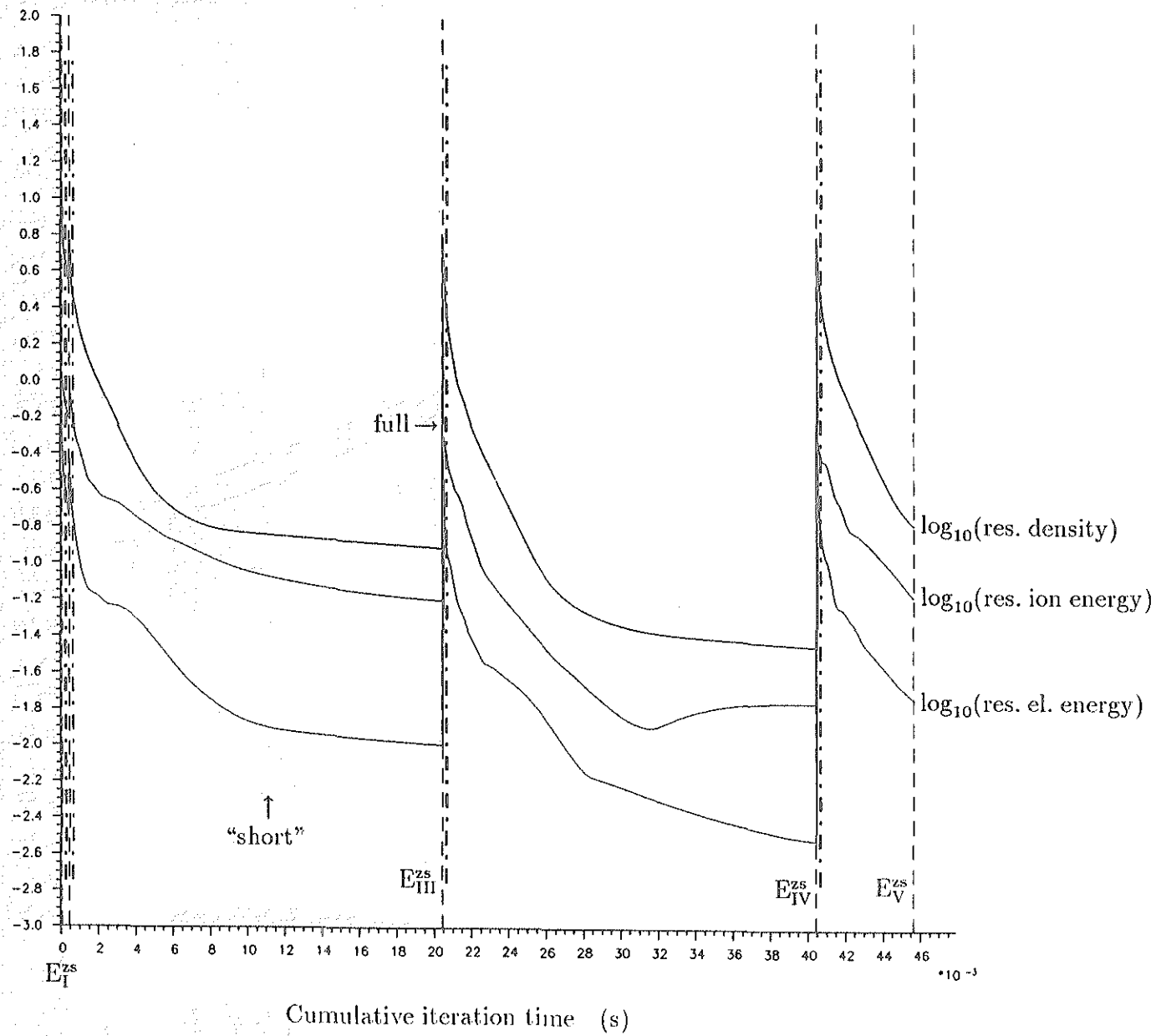


Fig.4 Perturbation of relaxed state – Hotston recycling

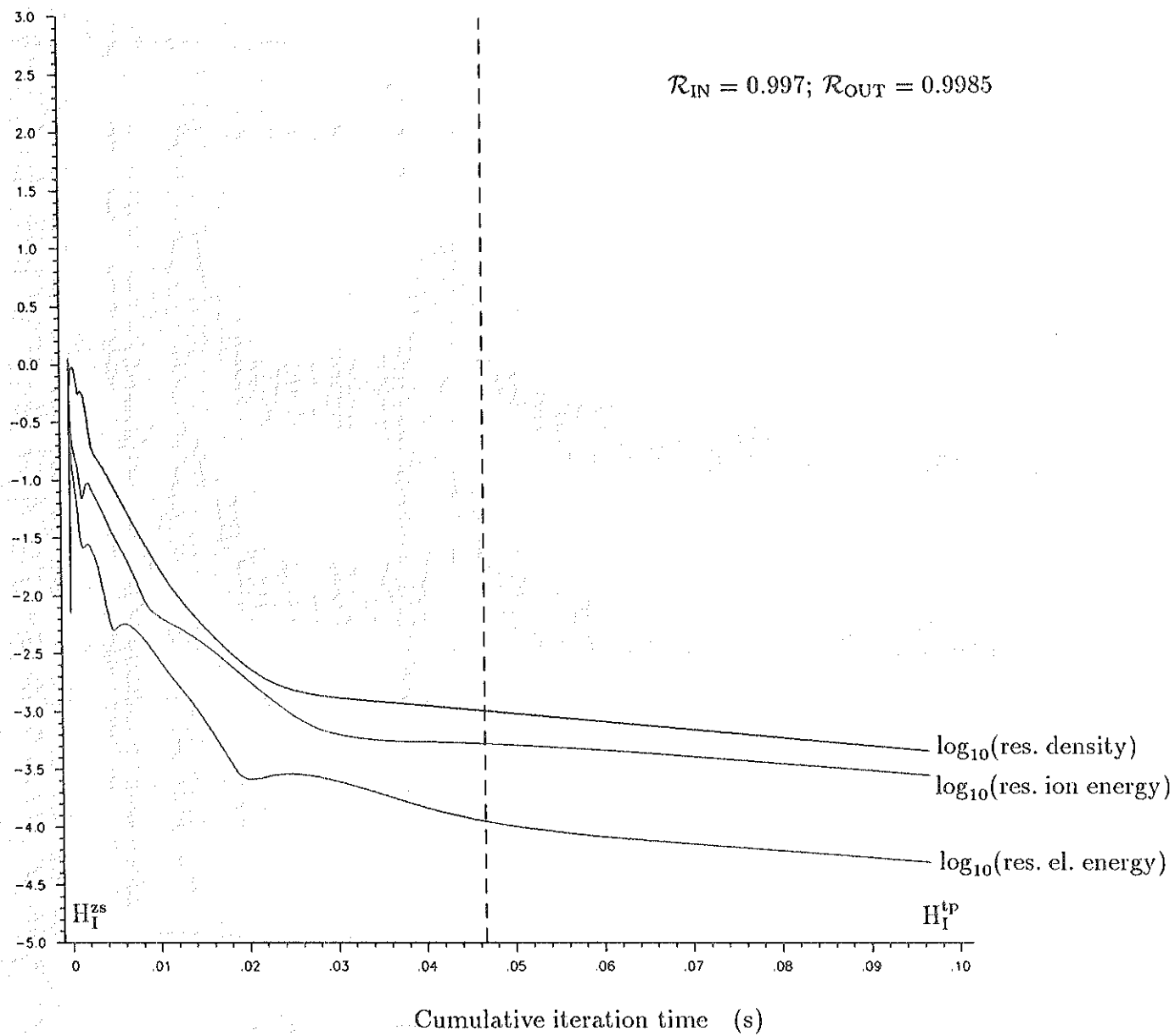


Fig.5 "B2"+EIRENE cycles - excessive time-step

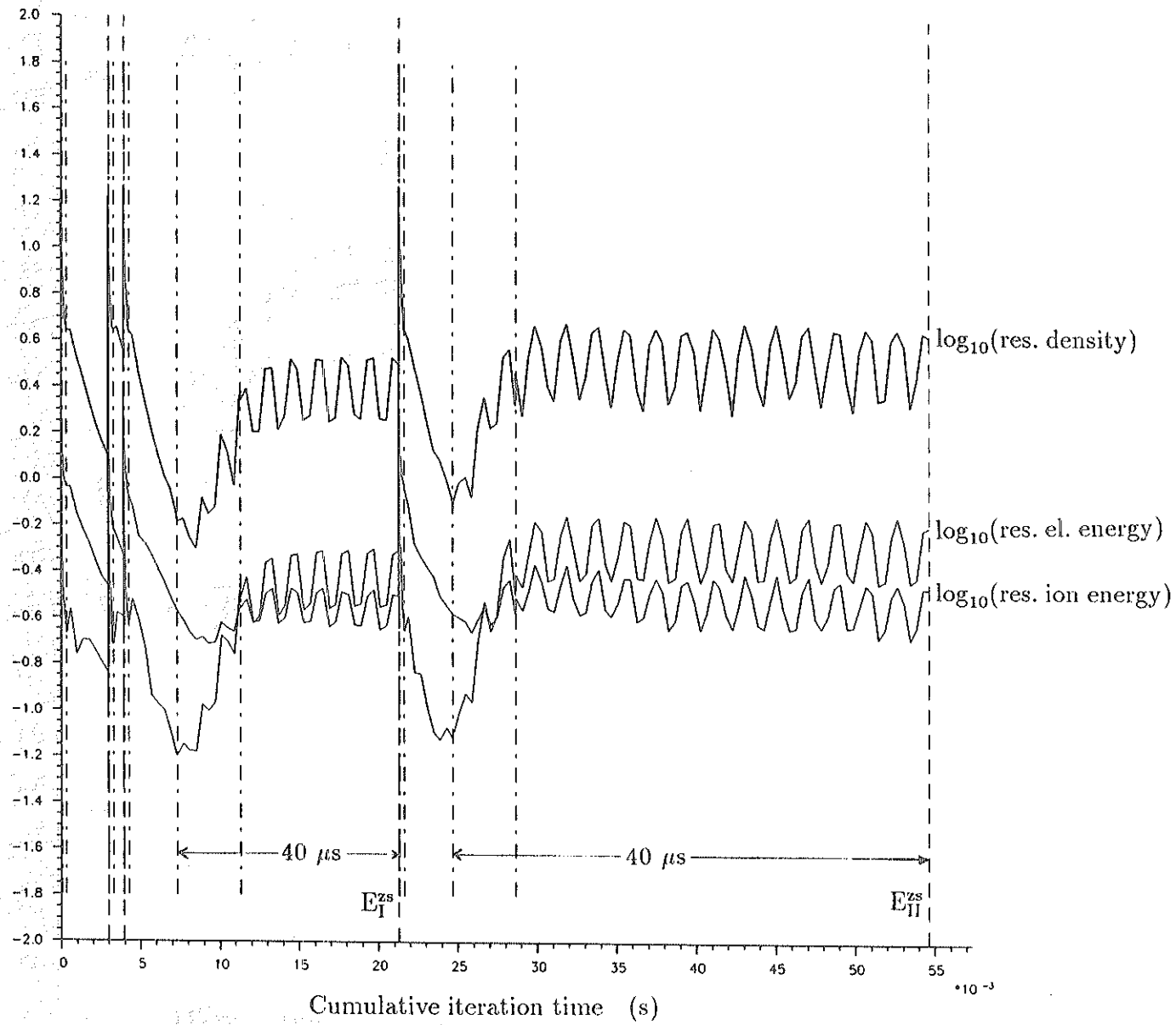


Fig.6 "B2"+EIRENE cycles – global balance errors

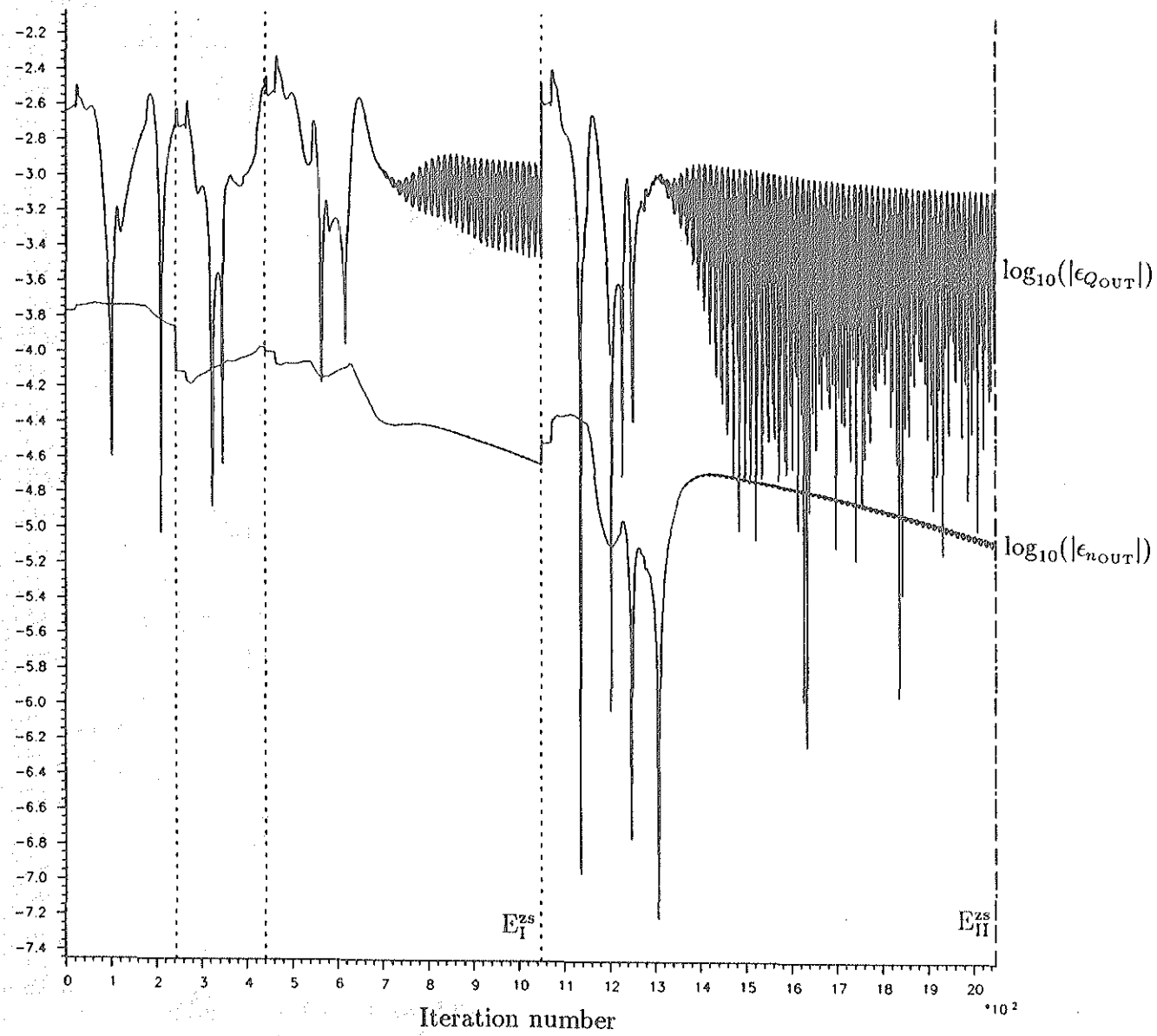


Fig.7 "B2"+EIRENE cycles - reduced time-step

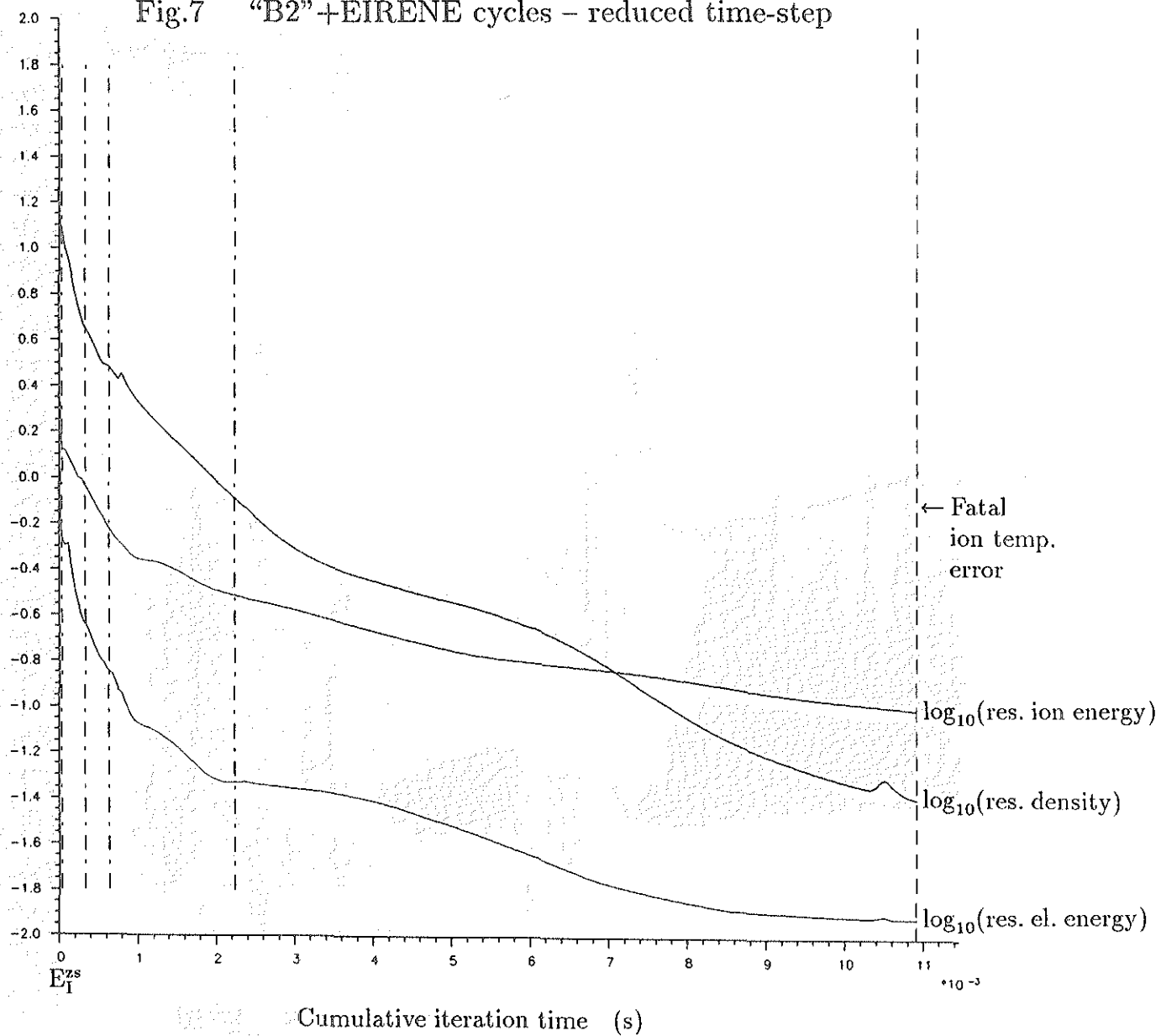


Fig.8 Evolution of “B2” residuals – “minimal” recycling

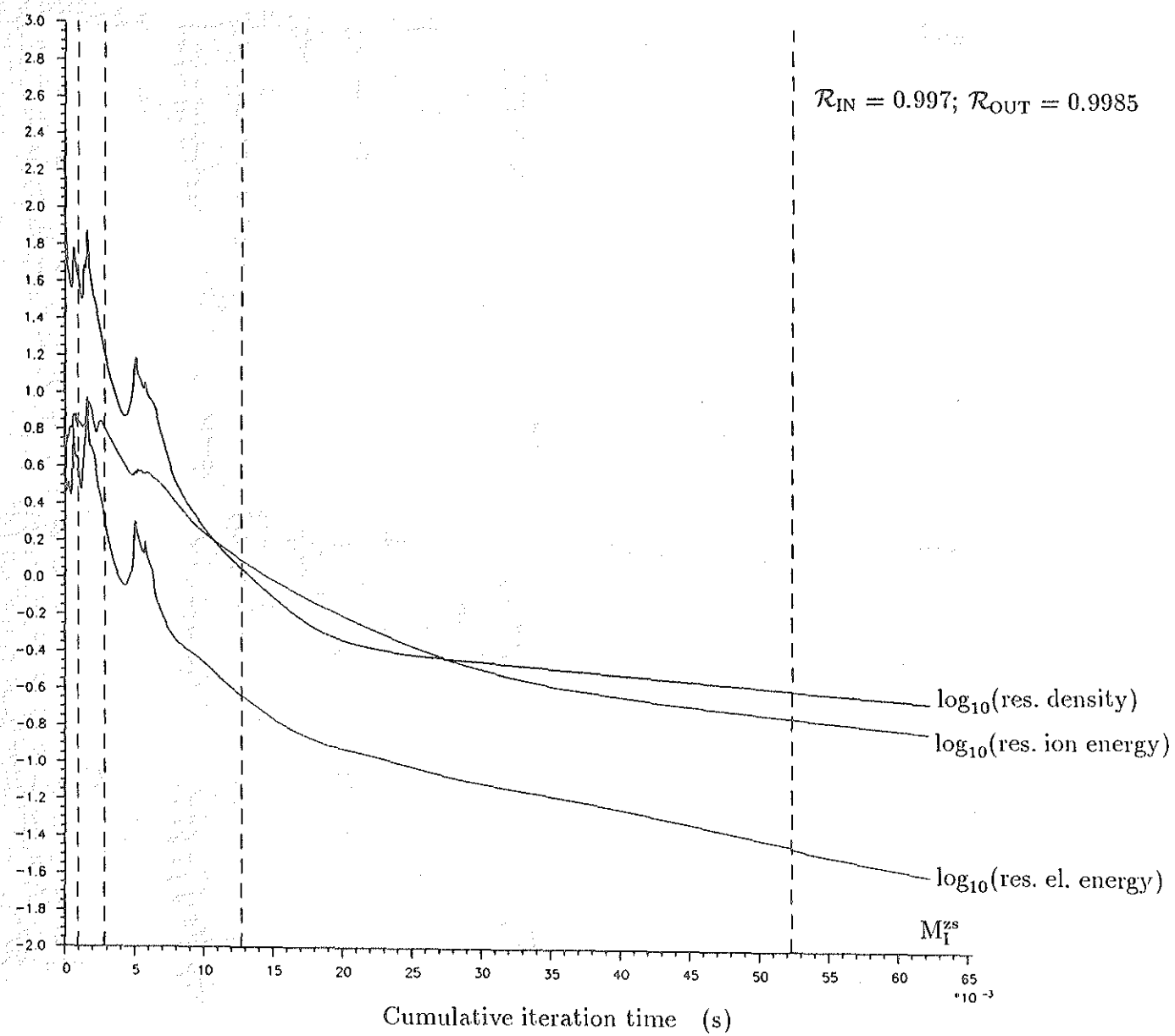


Fig.9 Jointly-normalized ion source per grid cell
 – different models for plasma H_I^{zs}
 ($\log_{10}(\text{source})$ v grid column index (ix), in each grid row (iy))

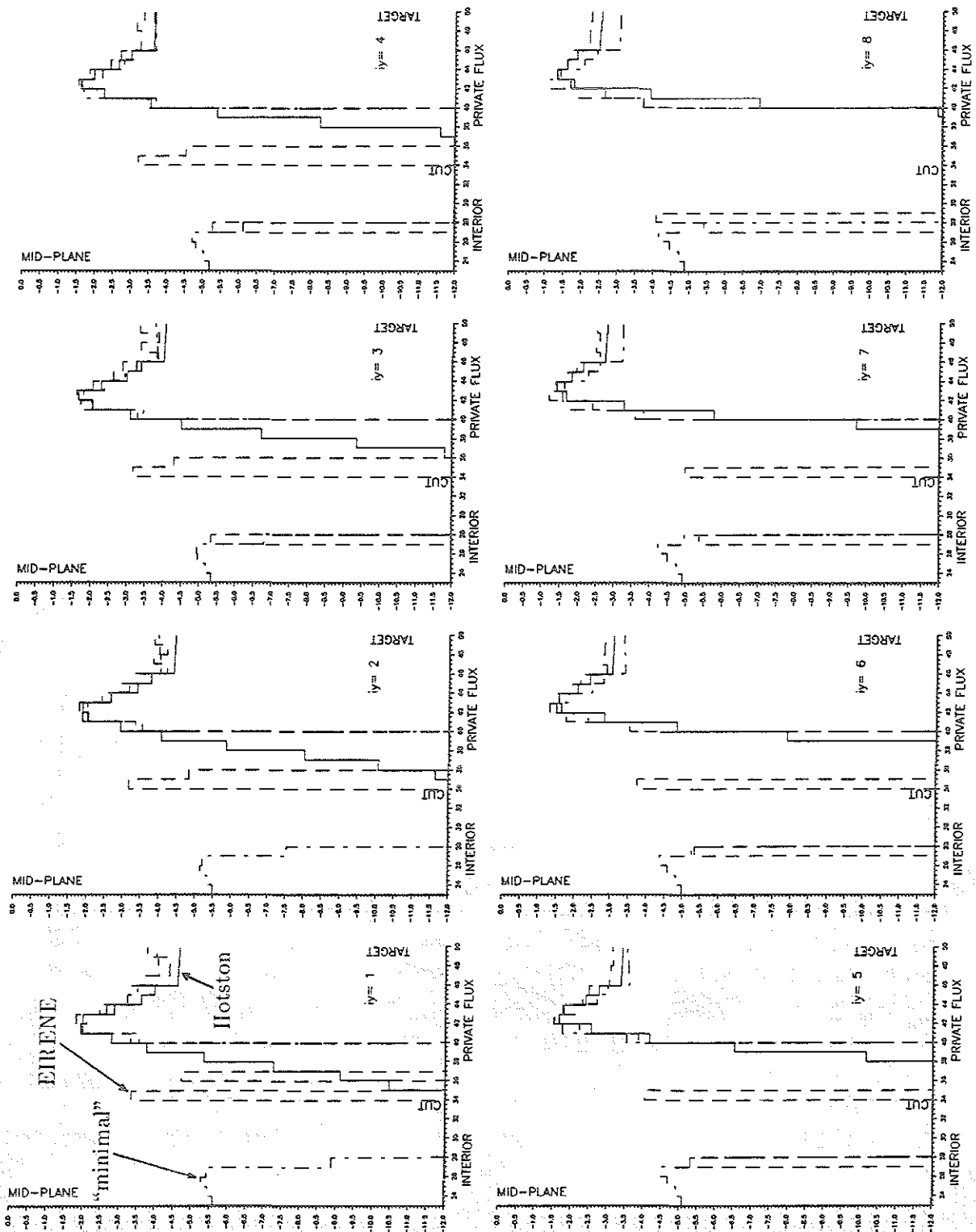


Fig.9 contd...

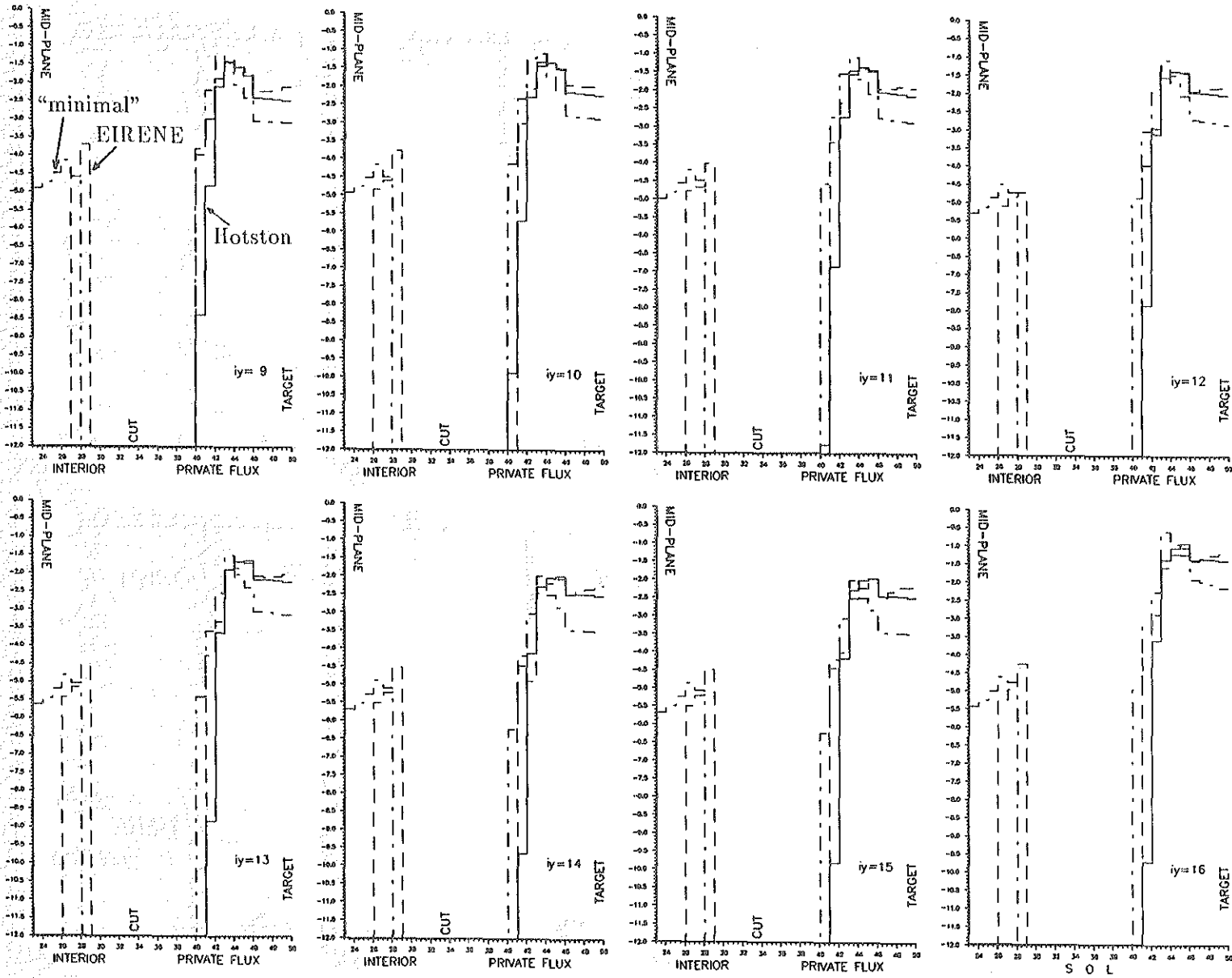
(separatrix between rows $i_y = 15$ and $i_y = 16$)

Fig.9 contd...

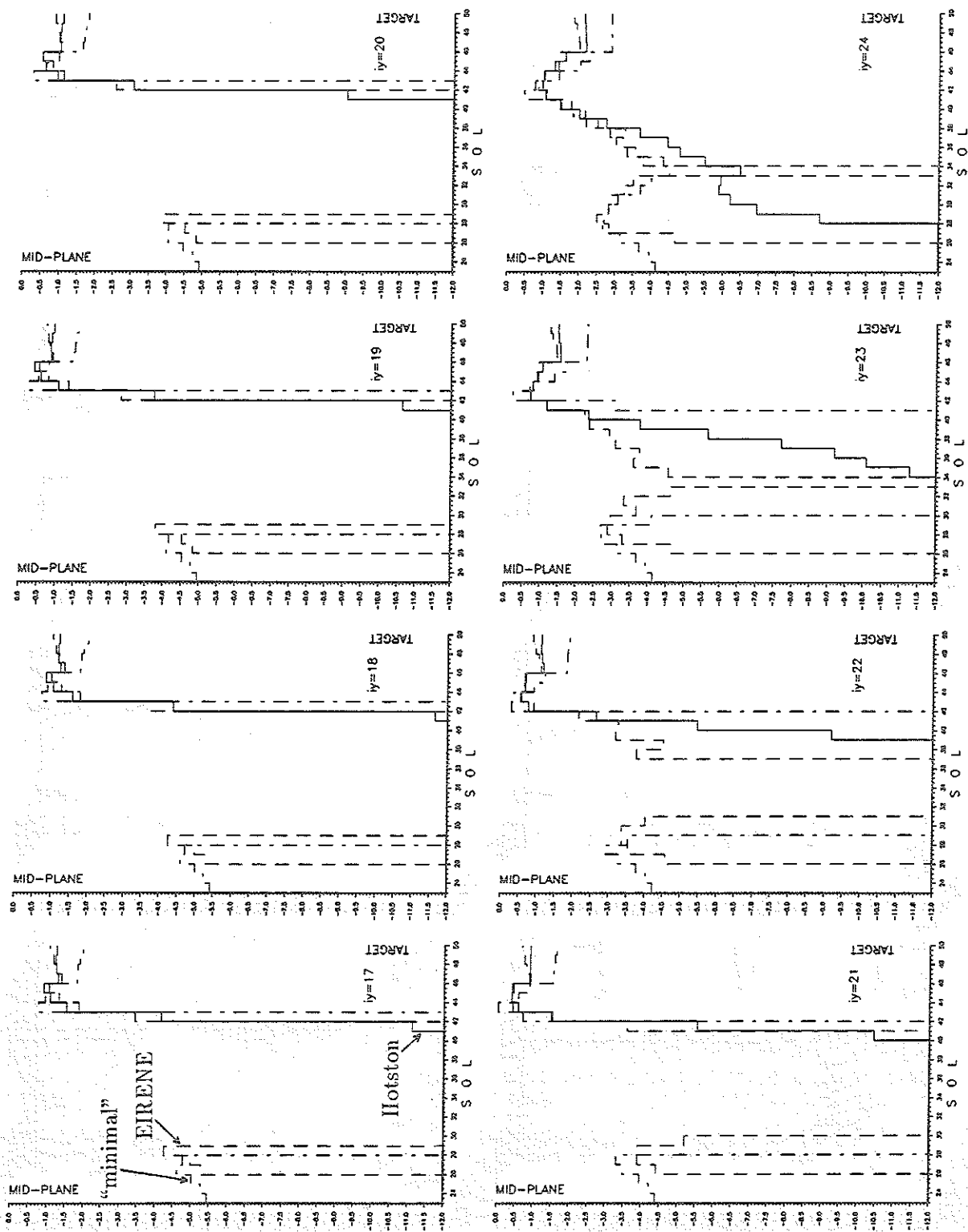


Fig.9 contd...

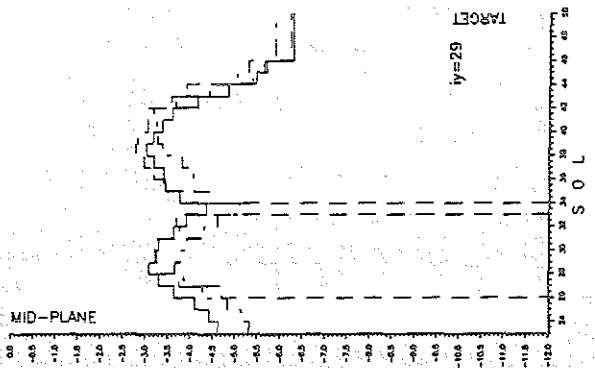
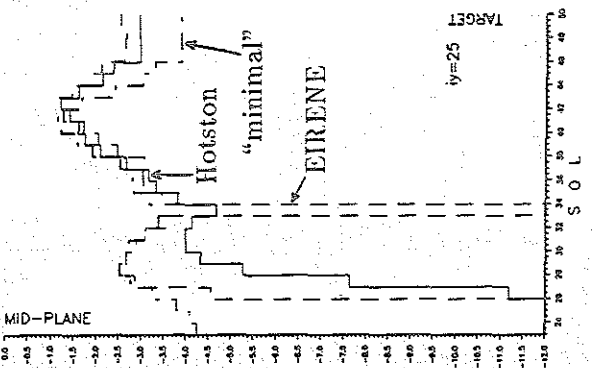
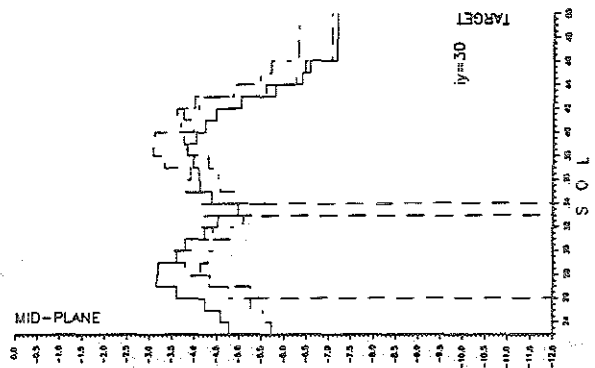
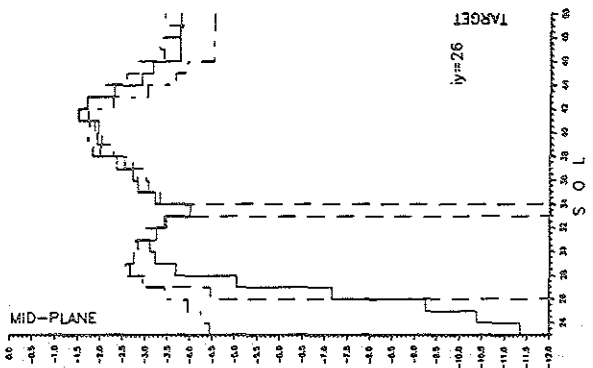
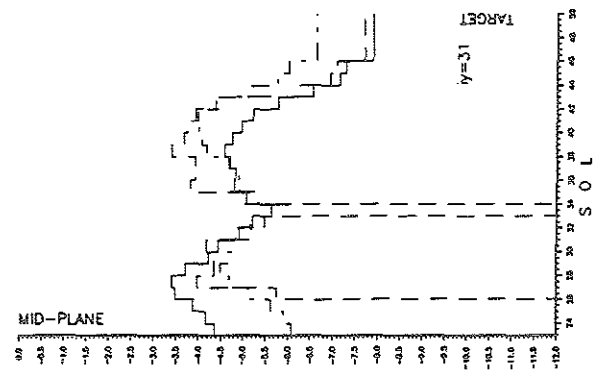
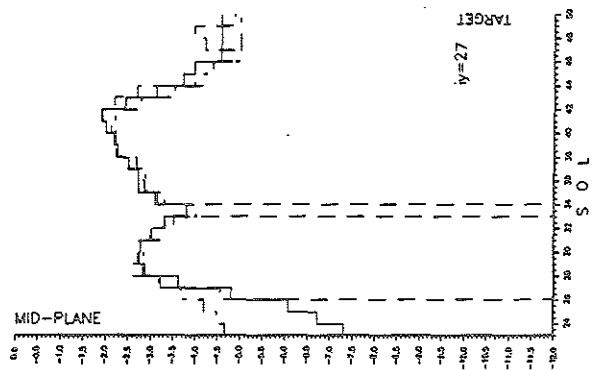
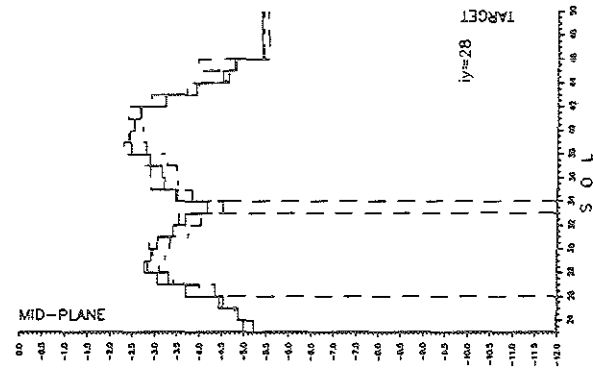
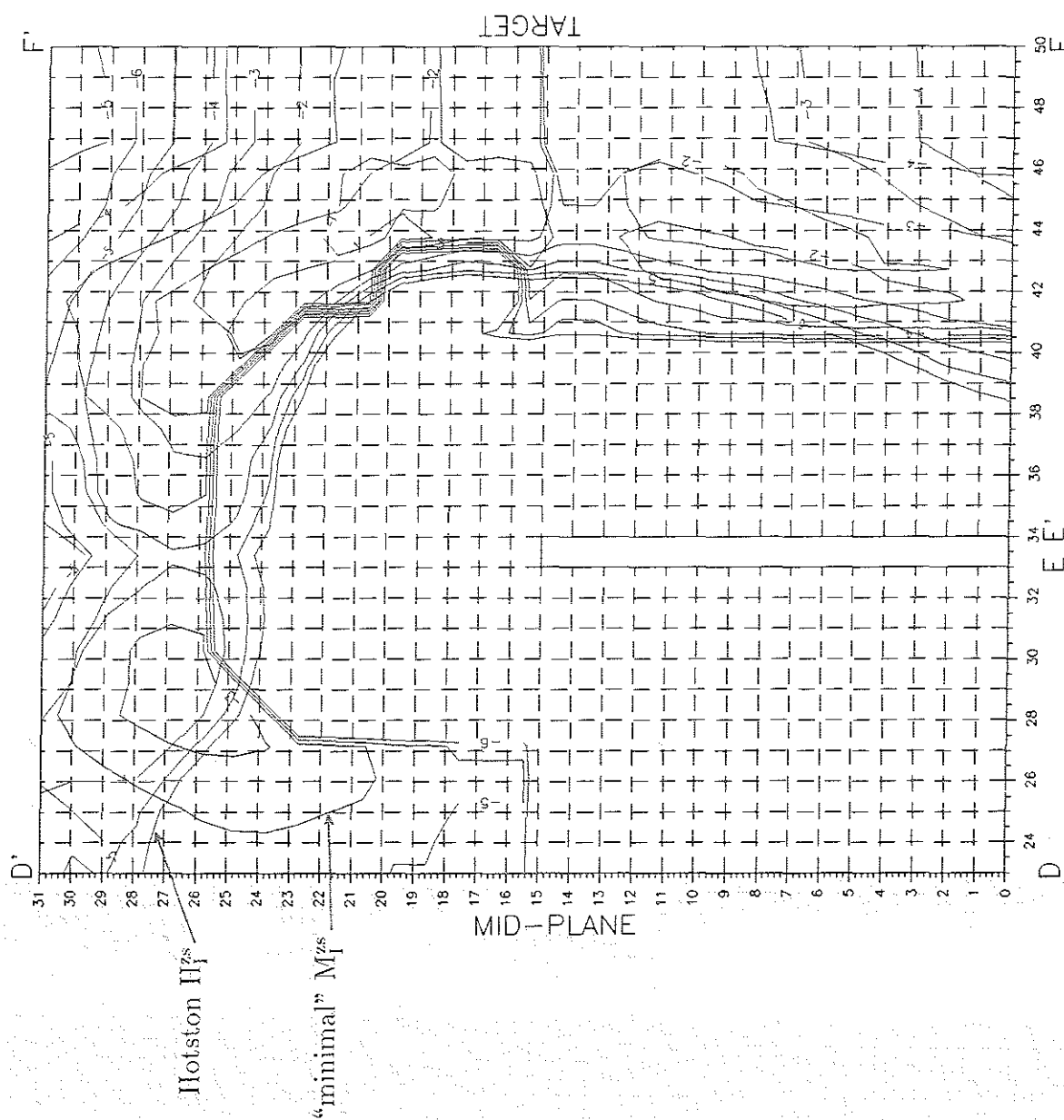


Fig.10 Jointly-normalized ion source per grid cell
 - Hotston state H_I^{zs} and "minimal" state M_I^{zs}
 (contours at 10^{-1} ; 10^{-2} ; ...; 10^{-6} , over grid cells)



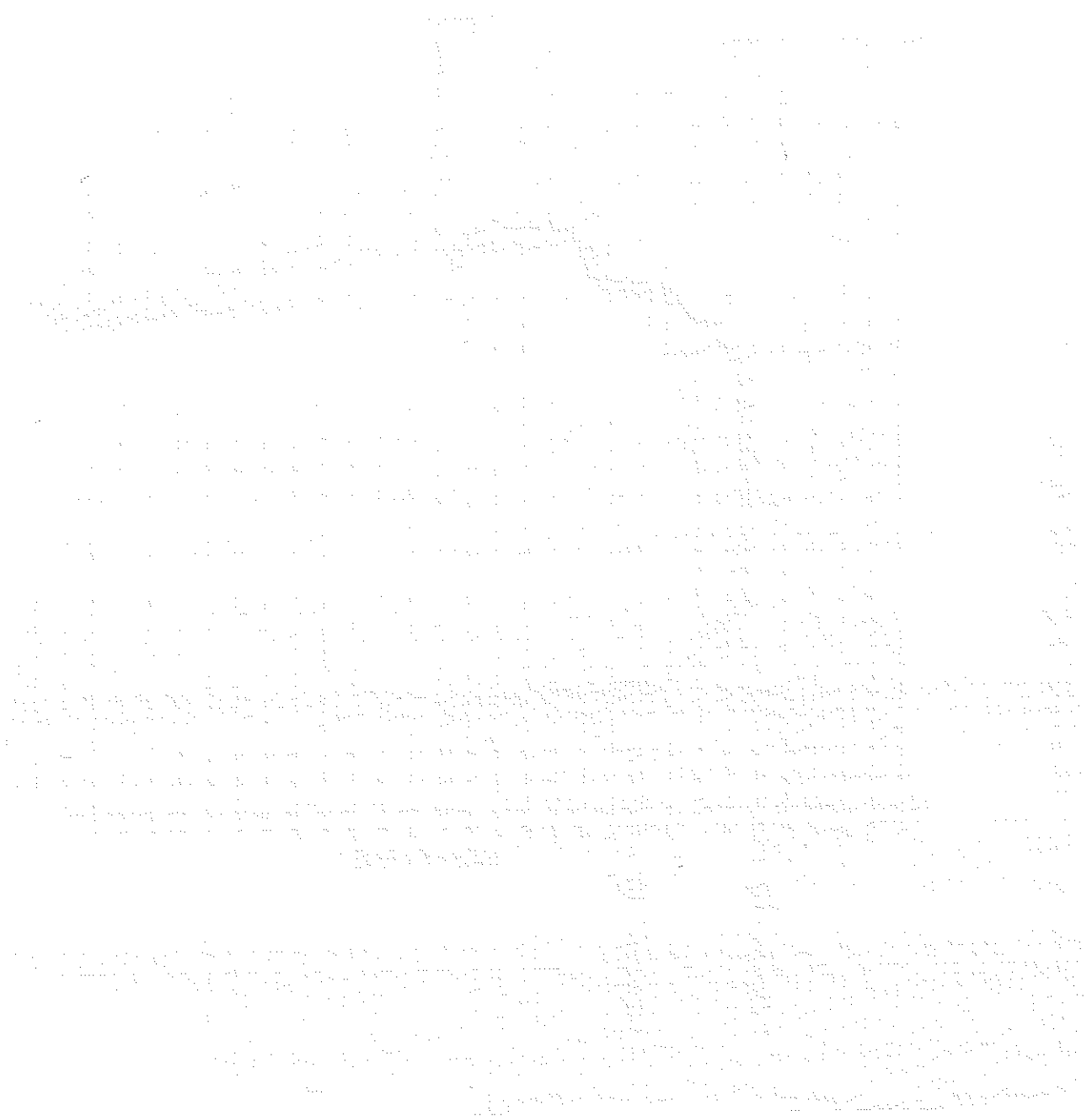


Fig.11 Switch from Hotston to "minimal" recycling

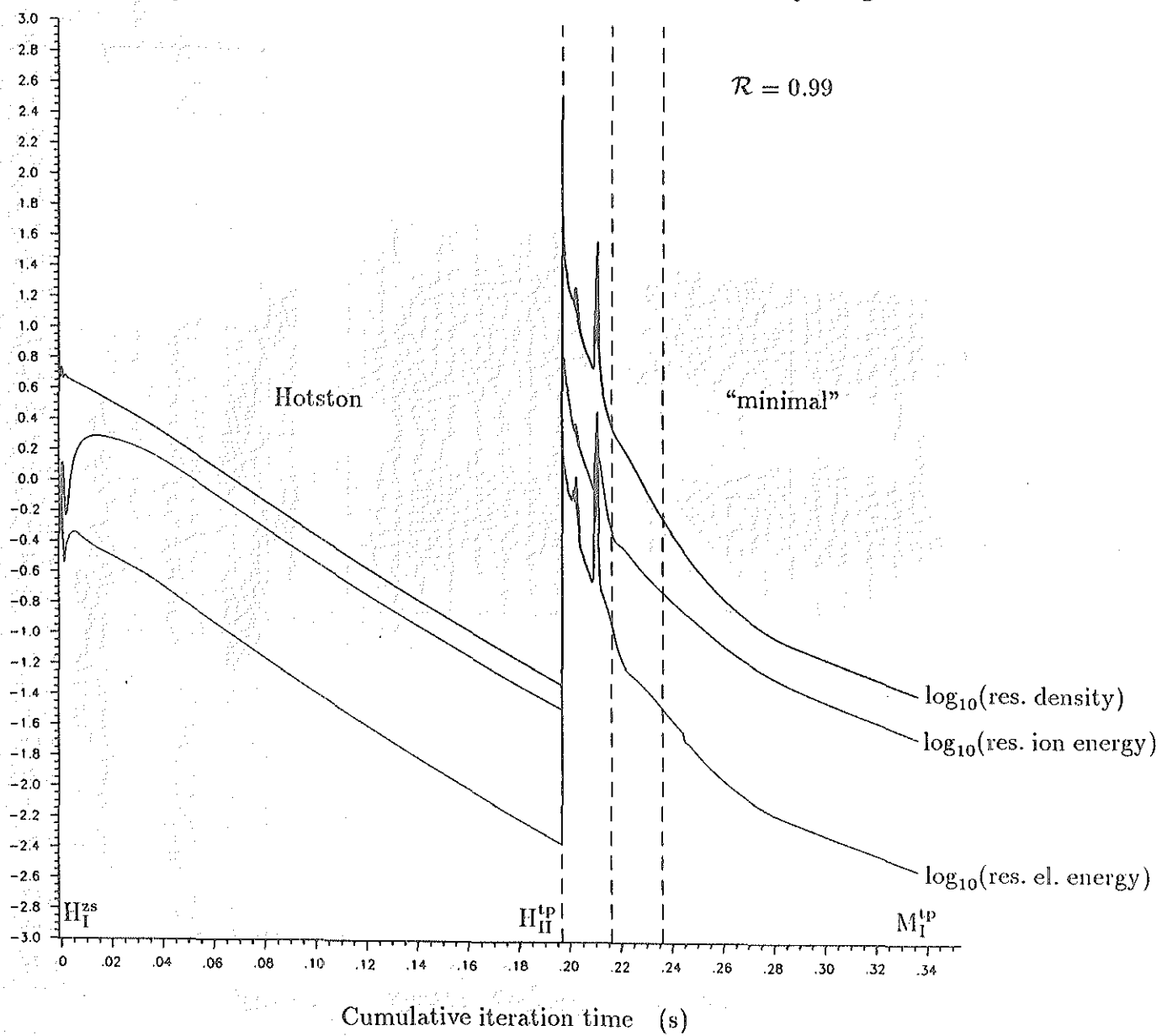


Fig.12 Intrinsic oscillation of "B2" residuals
- "minimal" recycling

$$\mathcal{R} = 0.98$$

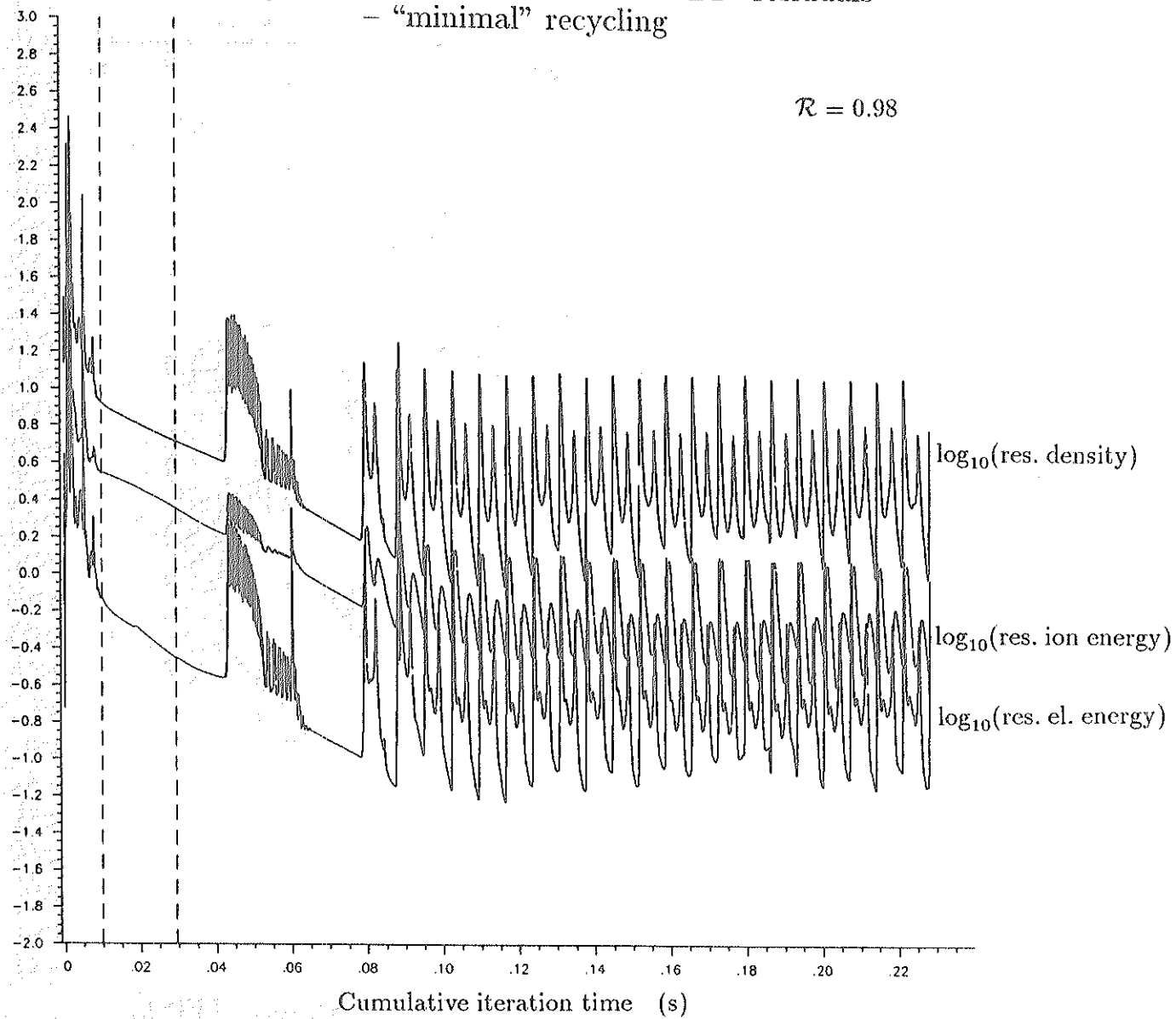
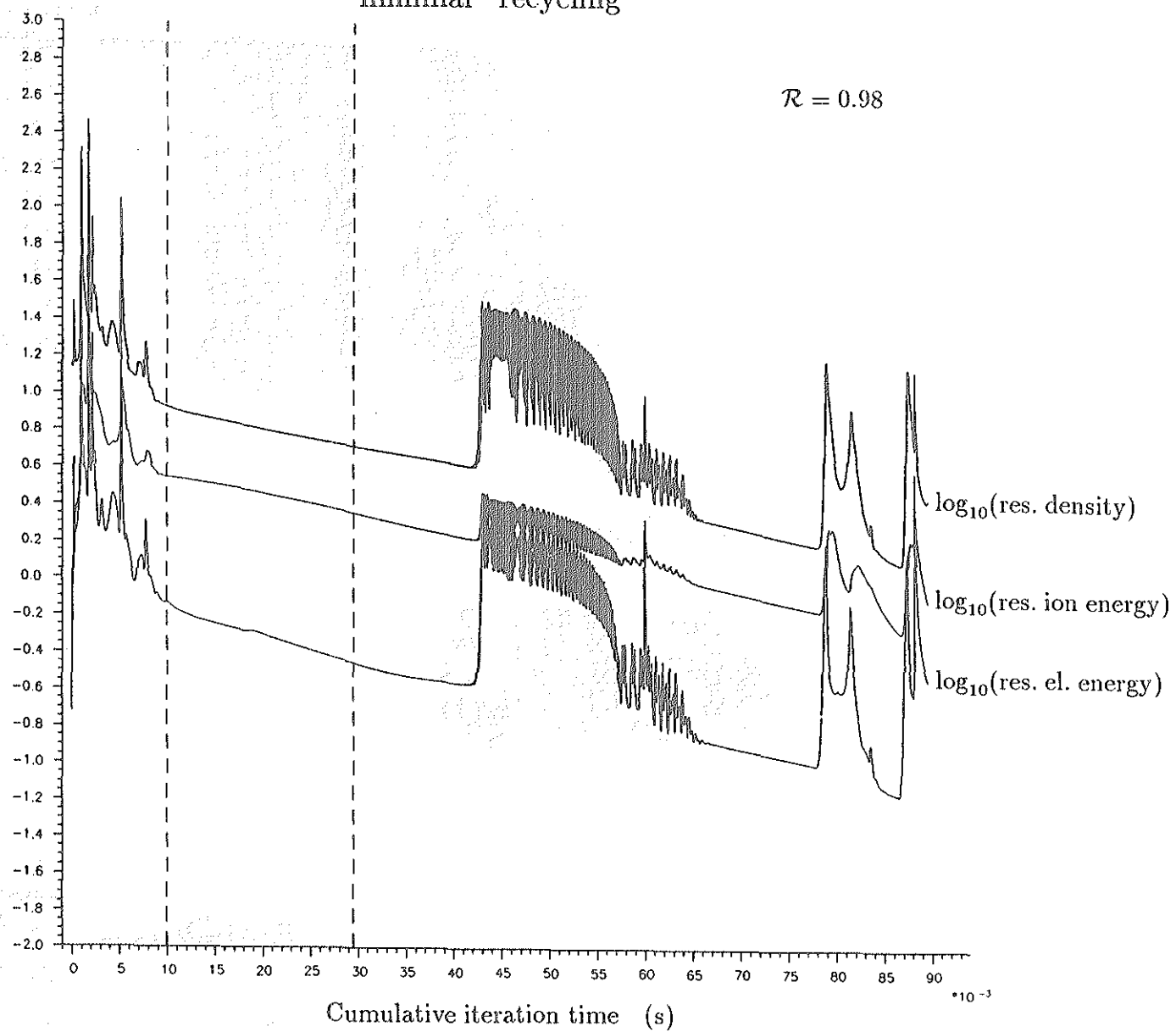
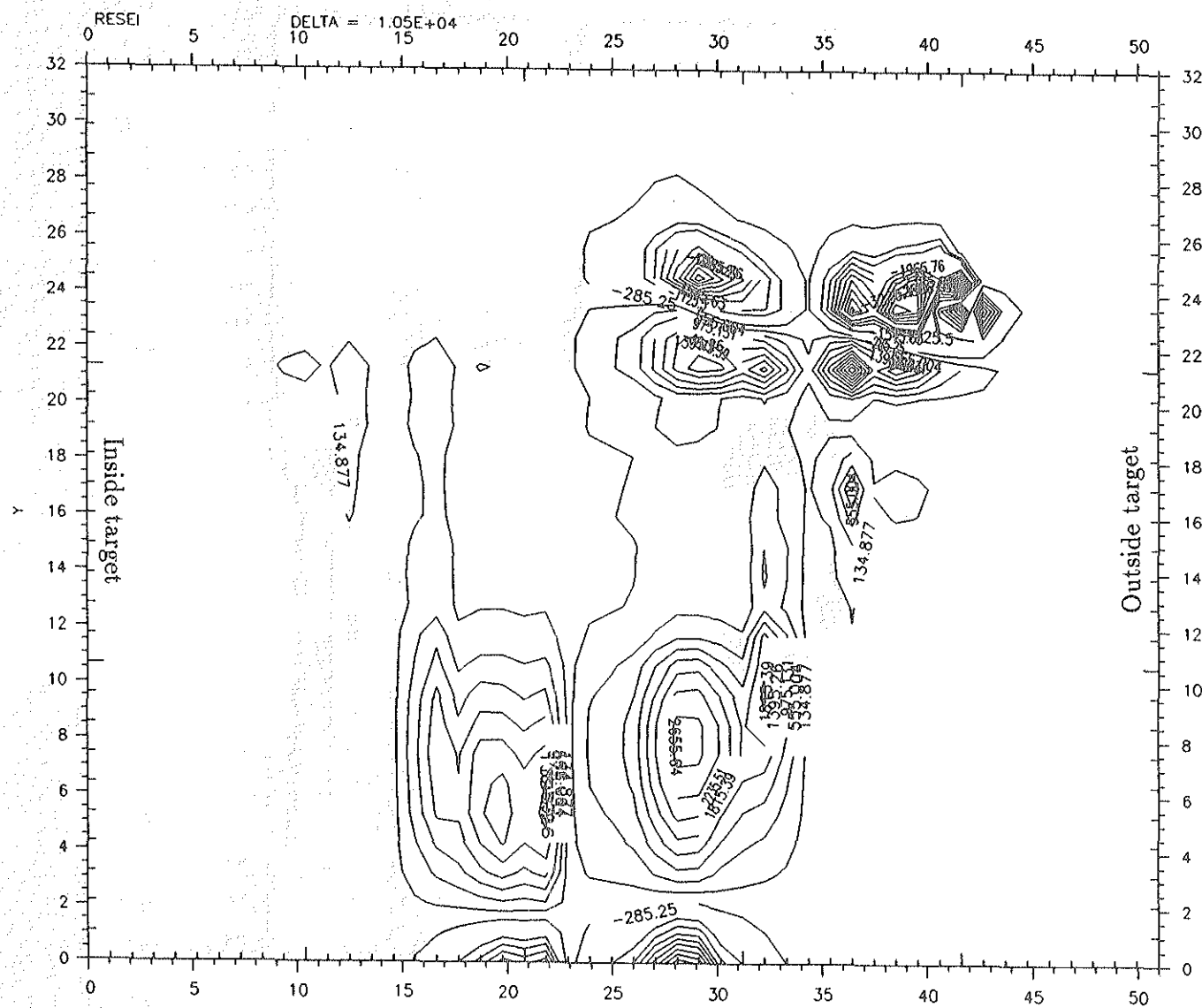


Fig.13 Intrinsic oscillation – reduced time-step
– “minimal” recycling



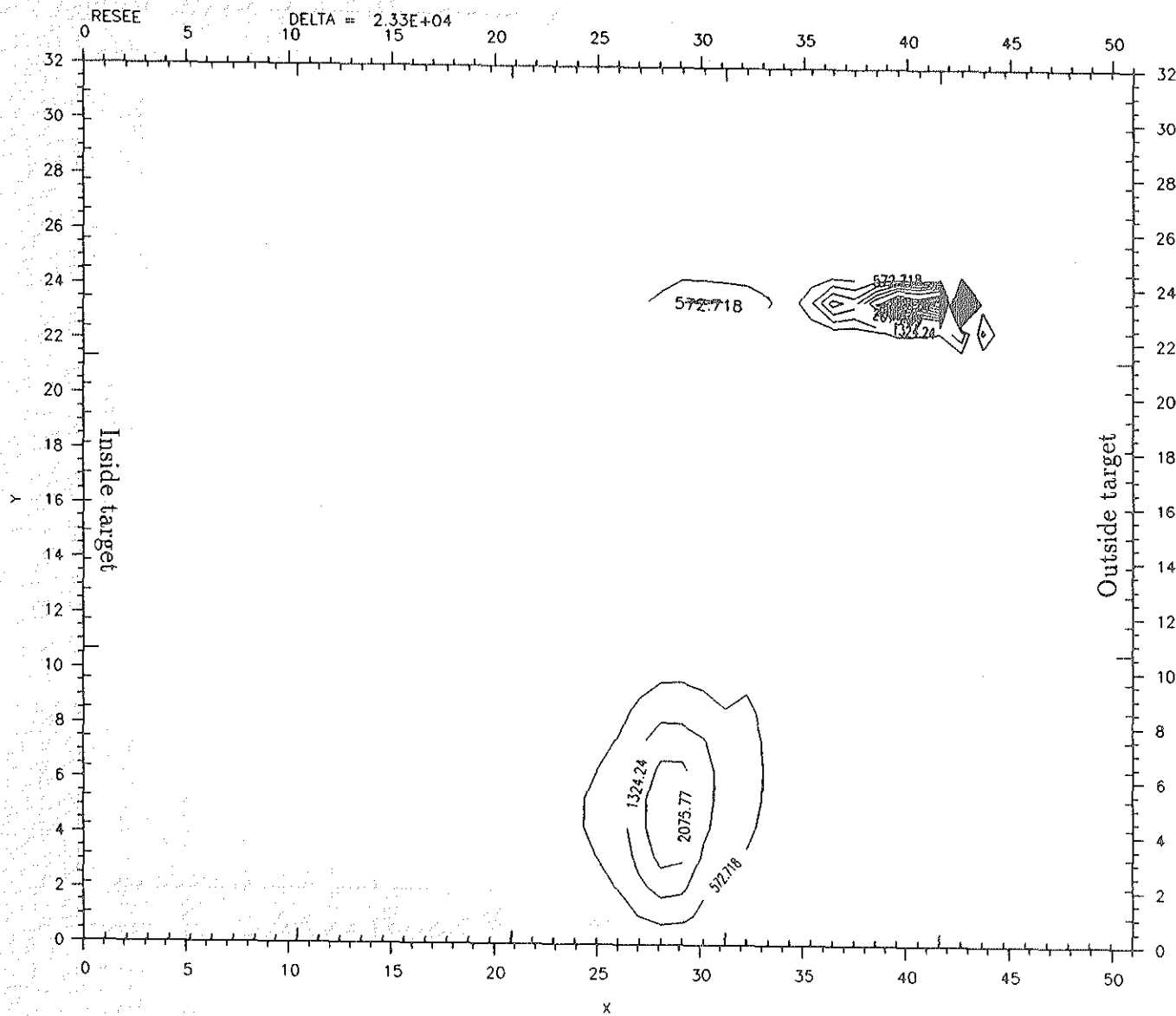


MIN: WERT = -5746.9
LAGE =(37,22)

MAX: WERT = 4336.14
LAGE =(35,20)

WERT	STRICH
-5746.9	_____
-5326.77	_____
-4906.64	_____
-4486.52	_____
-4066.39	_____
-3646.27	_____
-3226.14	_____
-2806.01	_____
-2385.89	_____
-1965.76	_____
-1545.63	_____
-1125.5	_____
-705.377	_____
-285.25	_____
134.877	_____
555.004	_____
975.131	_____
1395.26	_____
1815.39	_____
2235.51	_____
2655.64	_____
3075.77	_____
3495.89	_____
3916.02	_____
4336.14	_____

Fig.14 Local "B2" residuals over all grid cells
- at conclusion of Fig.13
(i) ion energy residual

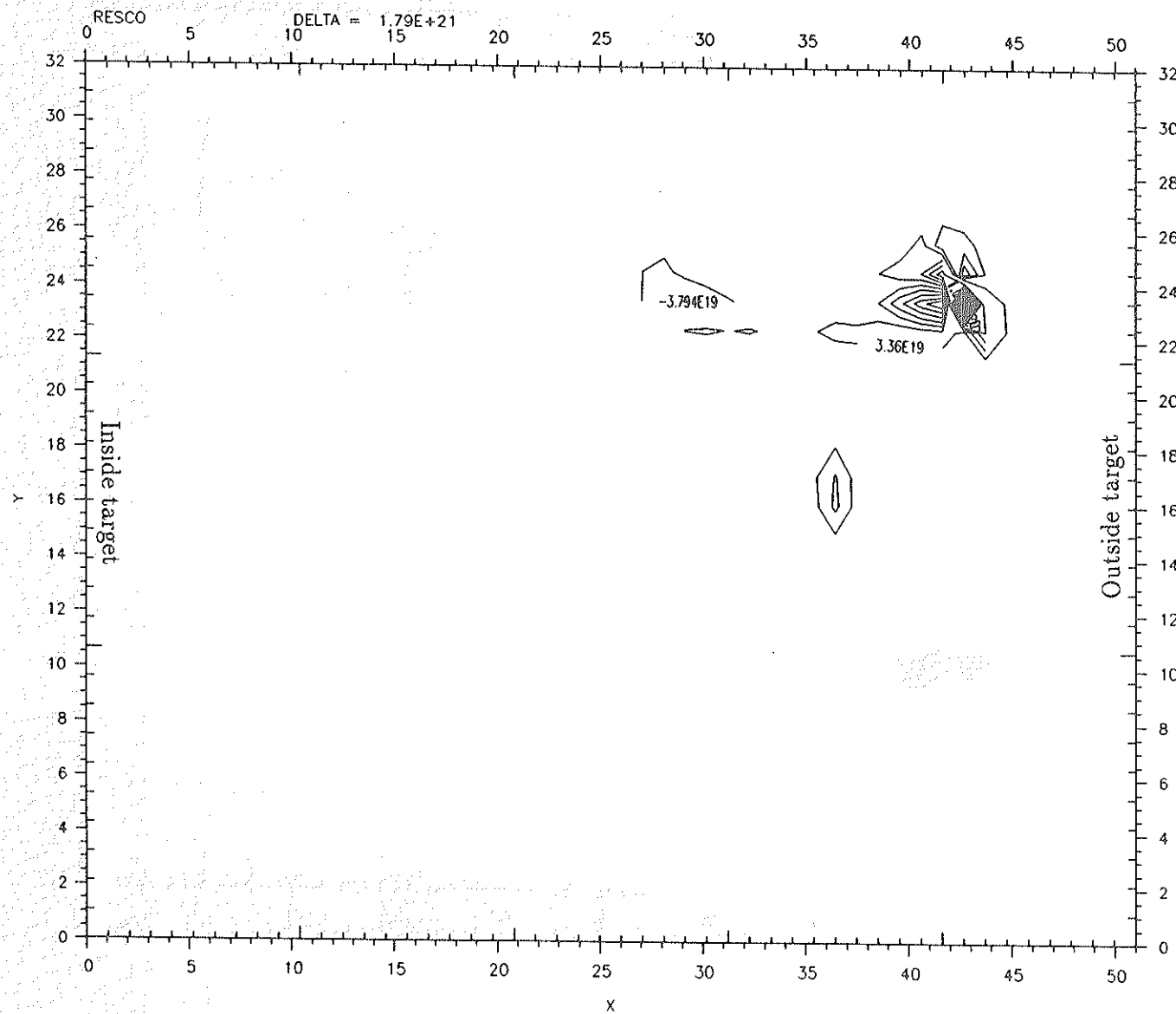


MIN: WERT = -9197.09
LAGE = (41,22)

MAX: WERT = 8839.48
LAGE = (40,22)

WERT	STRICH
-9197.09	_____
-8445.57	_____
-7694.05	_____
-6942.52	_____
-6191.	_____
-5439.47	_____
-4687.95	_____
-3936.43	_____
-3184.9	_____
-2433.38	_____
-1681.85	_____
-930.33	_____
-178.806	_____
572.718	_____
1324.24	_____
2075.77	_____
2827.29	_____
3578.81	_____
4330.34	_____
5081.86	_____
5833.39	_____
6584.91	_____
7336.43	_____
8087.96	_____
8839.48	_____

Fig.14 contd...
(ii) electron energy residual



MIN: WERT = $-3.956\text{E}20$
 LAGE = (40,22)

MAX: WERT = $1.321\text{E}21$
 LAGE = (41,22)

WERT	STRICH
$-3.956\text{E}20$	_____
$-3.241\text{E}20$	_____
$-2.526\text{E}20$	_____
$-1.81\text{E}20$	_____
$-1.095\text{E}20$	_____
$-3.794\text{E}19$	_____
$3.36\text{E}19$	_____
$1.051\text{E}20$	_____
$1.767\text{E}20$	_____
$2.482\text{E}20$	_____
$3.198\text{E}20$	_____
$3.913\text{E}20$	_____
$4.628\text{E}20$	_____
$5.344\text{E}20$	_____
$6.059\text{E}20$	_____
$6.775\text{E}20$	_____
$7.49\text{E}20$	_____
$8.205\text{E}20$	_____
$8.921\text{E}20$	_____
$9.636\text{E}20$	_____
$1.035\text{E}21$	_____
$1.107\text{E}21$	_____
$1.178\text{E}21$	_____
$1.25\text{E}21$	_____
$1.321\text{E}21$	_____

Fig.14 contd...
 (iii) density residual

Fig.15 Intrinsic oscillation – altered starting condition
– Hotston to “minimal” recycling

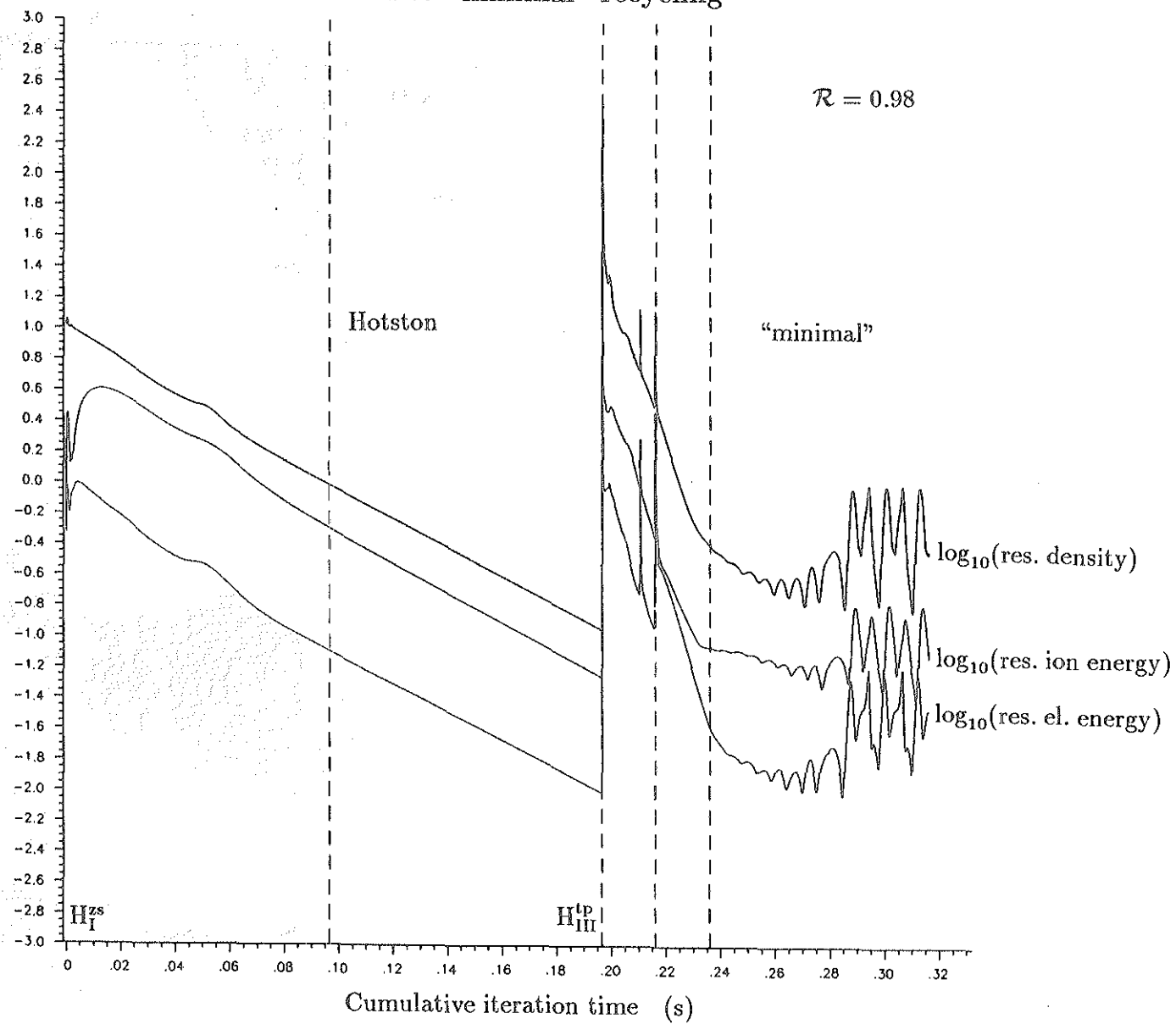
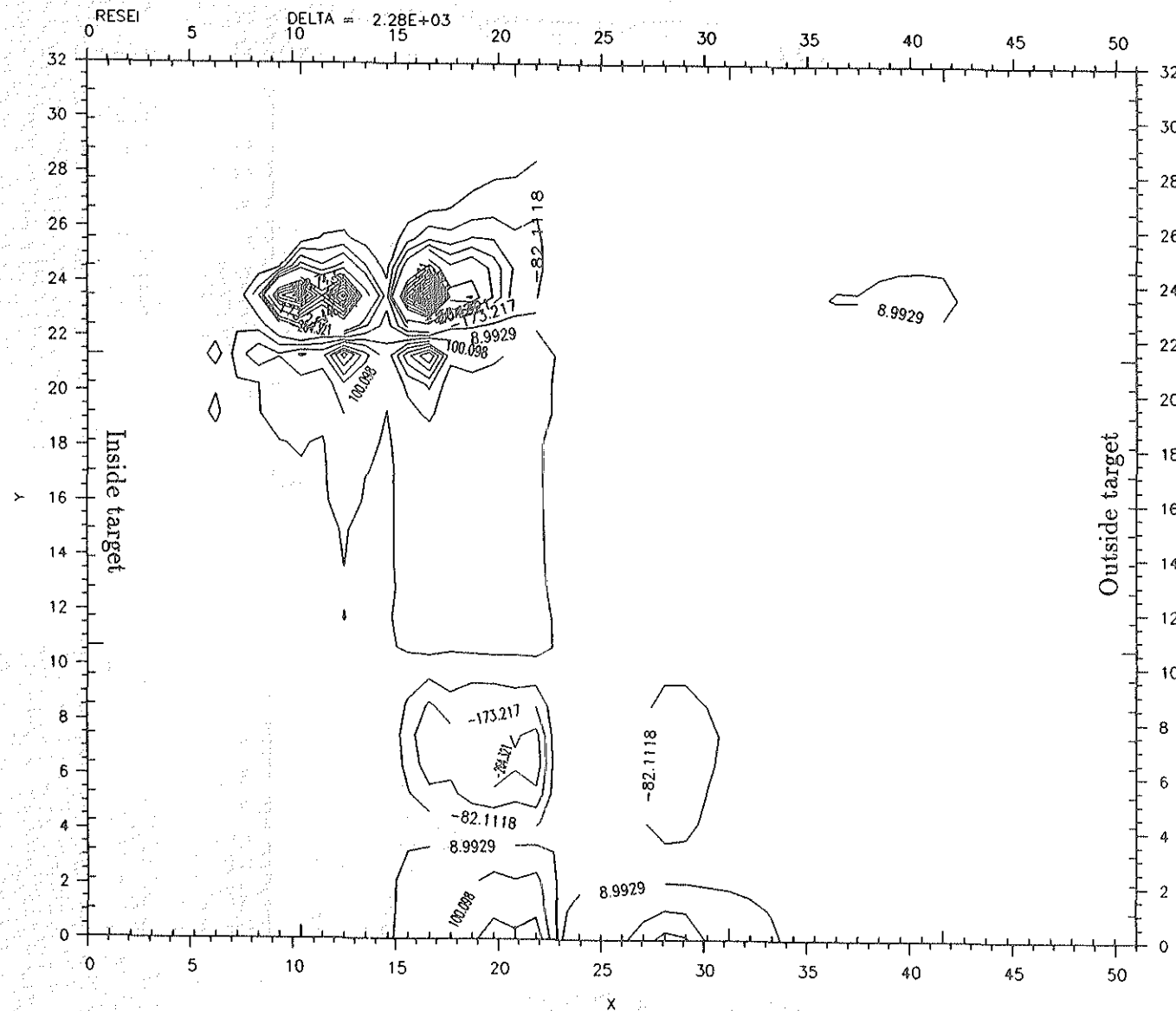
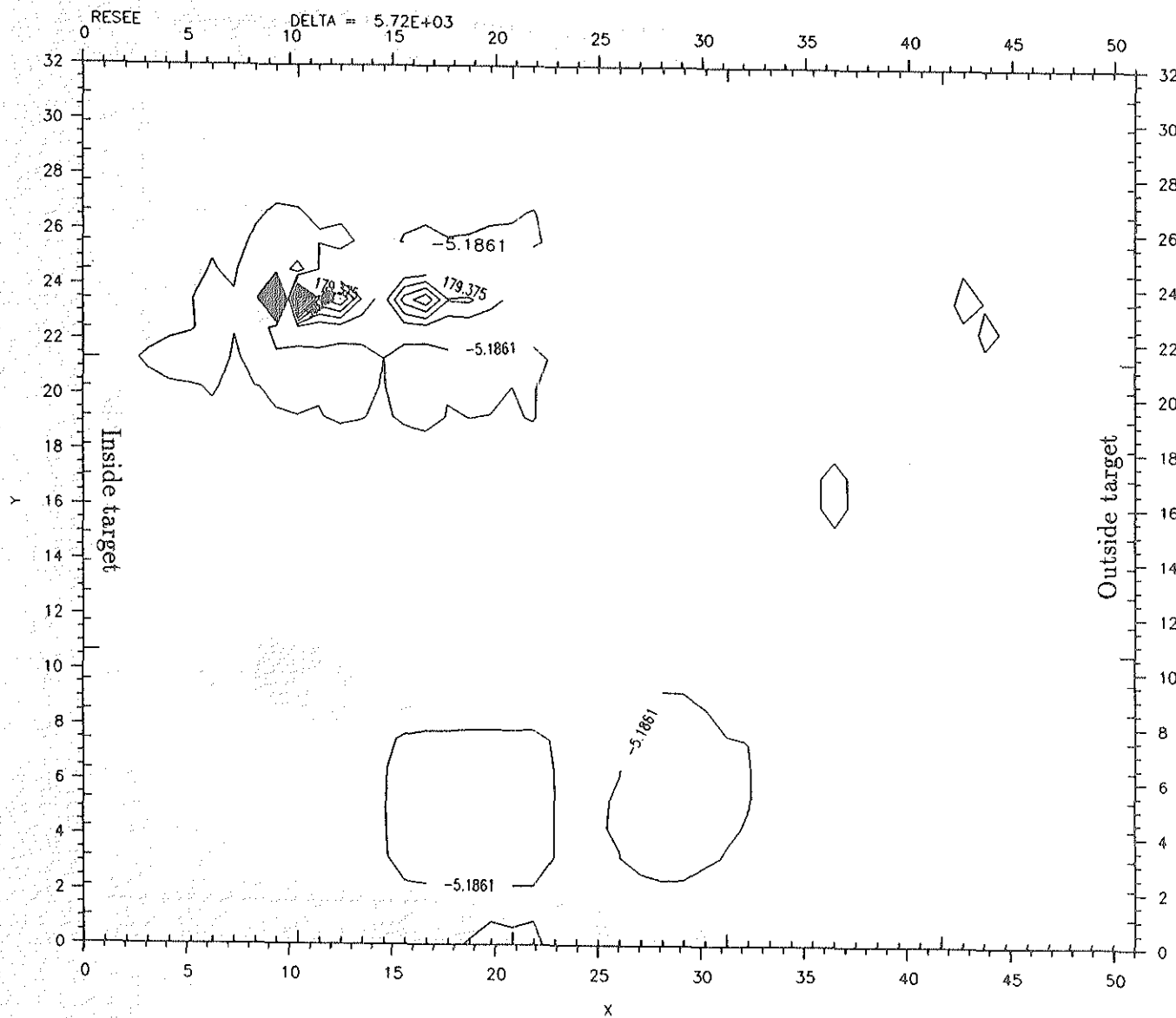


Fig.16 Local "B2" residuals over all grid cells
 - at conclusion of Fig.15
 (i) ion energy residual

MIN: WERT = -1630.89
 LAGE =(16,22)
 MAX: WERT = 555.621
 LAGE =(16,20)

WERT	STRICH
-1630.89	
-1539.79	
-1448.68	
-1357.58	
-1266.47	
-1175.37	
-1084.26	
-993.159	
-902.054	
-810.949	
-719.844	
-628.74	
-537.635	
-446.531	
-355.426	
-264.321	
-173.217	
-82.1118	
8.9929	
100.098	
191.202	
282.307	
373.412	
464.516	
555.621	



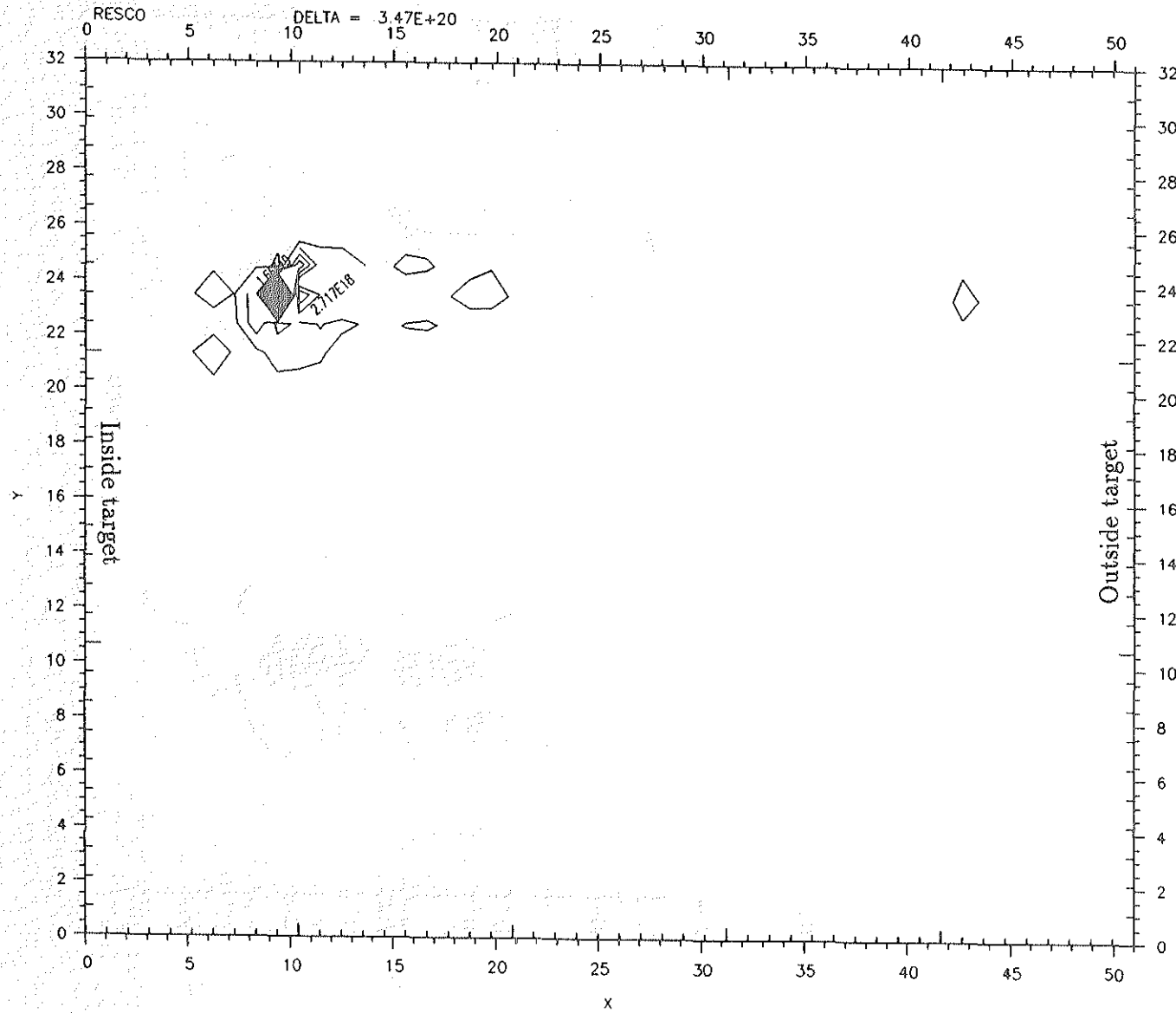


MIN: WERT = -2404.48
LAGE =(9,22)

MAX: WERT = 2024.98
LAGE =(10,22)

WERT	STRICH
-2404.48	_____
-2219.92	_____
-2035.36	_____
-1850.79	_____
-1666.23	_____
-1481.67	_____
-1297.11	_____
-1112.55	_____
-927.99	_____
-743.429	_____
-558.869	_____
-374.308	_____
-189.747	_____
-5.1861	_____
179.375	_____
363.936	_____
548.496	_____
733.057	_____
917.618	_____
1102.18	_____
1286.74	_____
1471.3	_____
1655.86	_____
1840.42	_____
2024.98	_____

Fig.16 contd...
(ii) electron energy residual



MIN: WERT = $-3.893E19$
 LAGE = (10,22)

MAX: WERT = $2.942E20$
 LAGE = (9,22)

WERT	STRICH
$-3.893E19$	_____
$-2.505E19$	_____
$-1.117E19$	_____
$2.717E18$	_____
$1.66E19$	_____
$3.048E19$	_____
$4.436E19$	_____
$5.824E19$	_____
$7.213E19$	_____
$8.601E19$	_____
$9.989E19$	_____
$1.138E20$	_____
$1.277E20$	_____
$1.415E20$	_____
$1.554E20$	_____
$1.693E20$	_____
$1.832E20$	_____
$1.971E20$	_____
$2.109E20$	_____
$2.248E20$	_____
$2.387E20$	_____
$2.526E20$	_____
$2.665E20$	_____
$2.804E20$	_____
$2.942E20$	_____

Fig.16 contd...
 (iii) density residual

Fig.17 Intrinsic oscillation – increased under-relaxation
– Hotston to “minimal” recycling

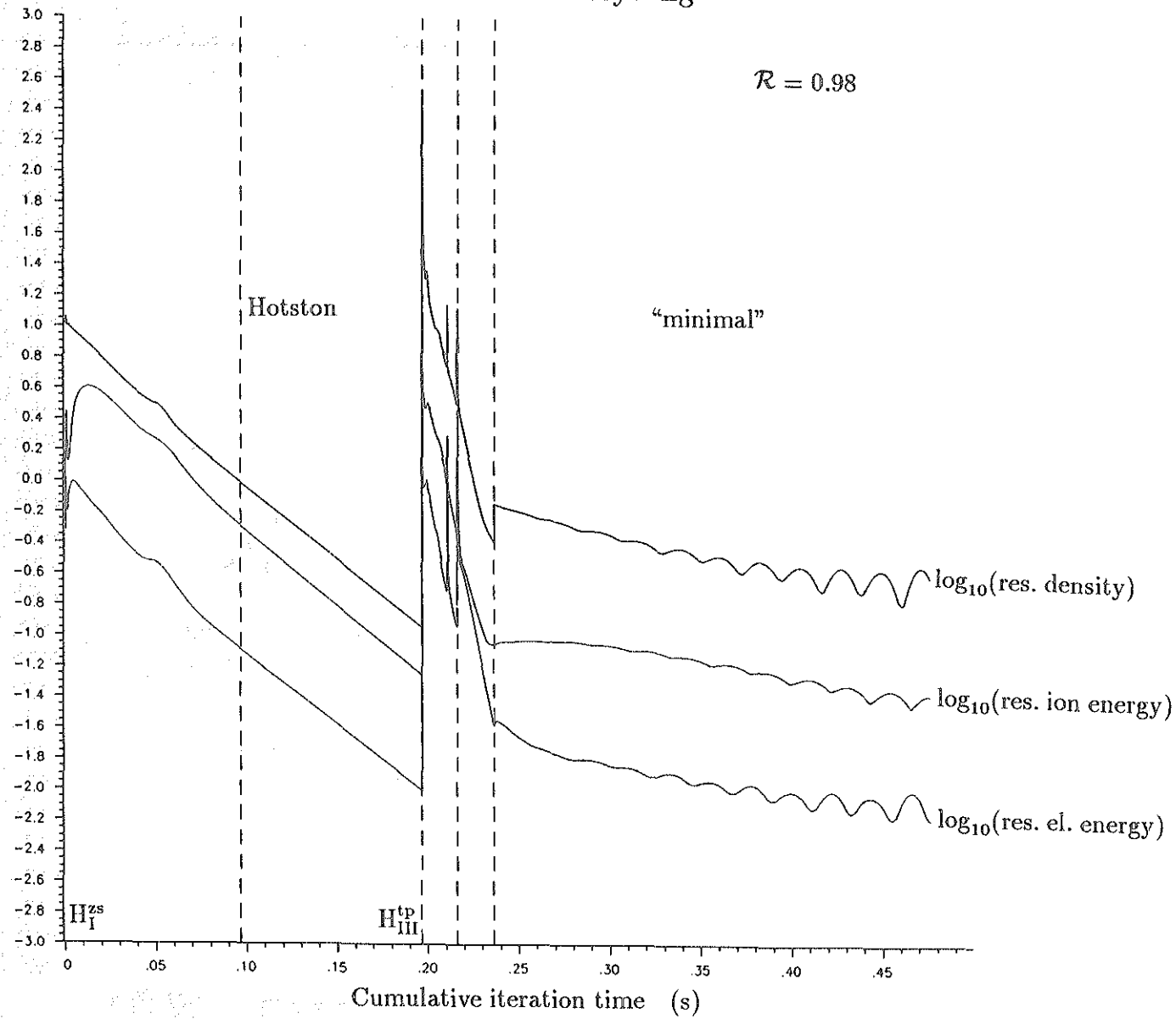


Fig.18 Evolution of "B2" residuals – Hotston recycling

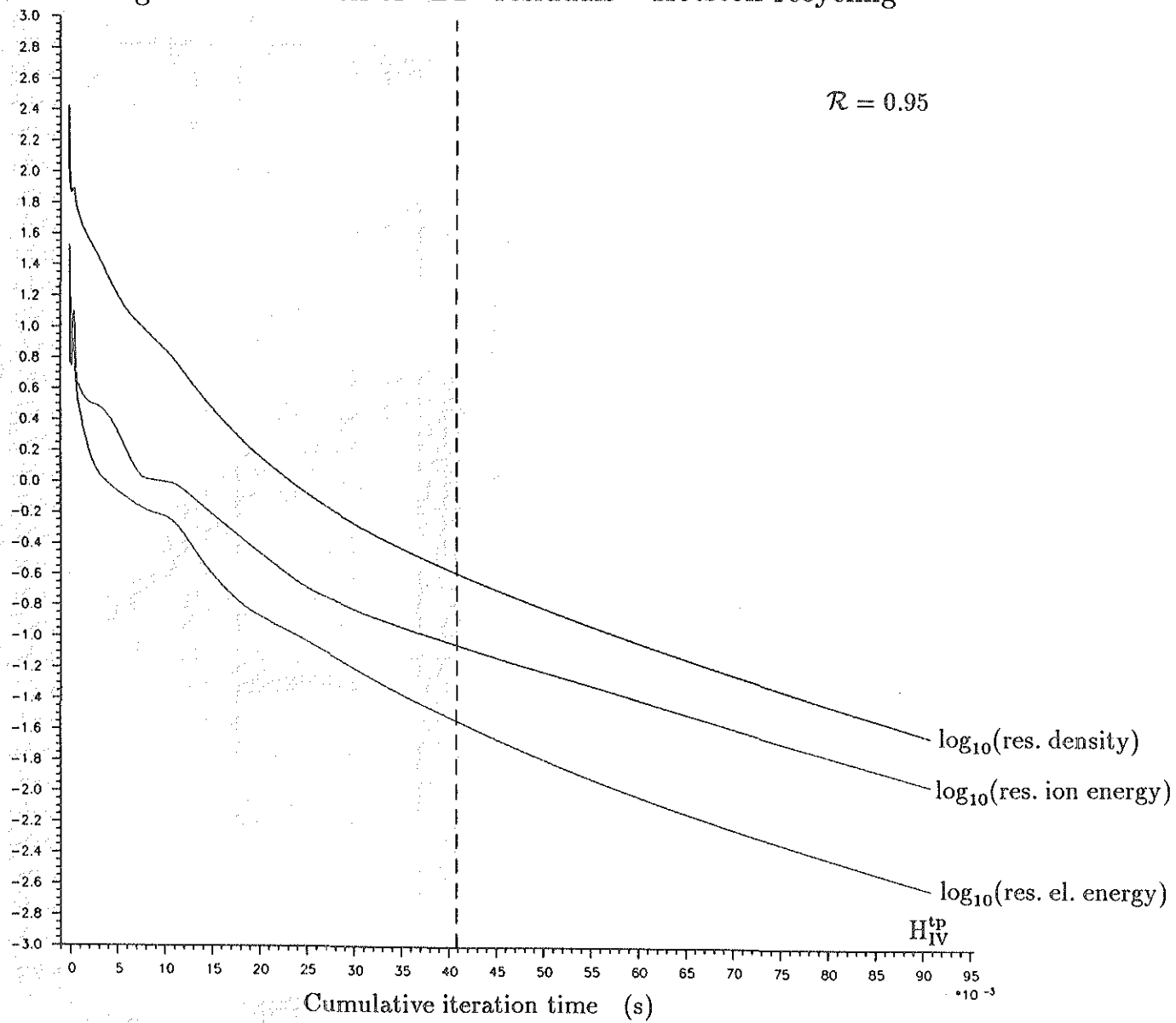


Fig.19 Decoupling of plasma balances – “minimal” recycling

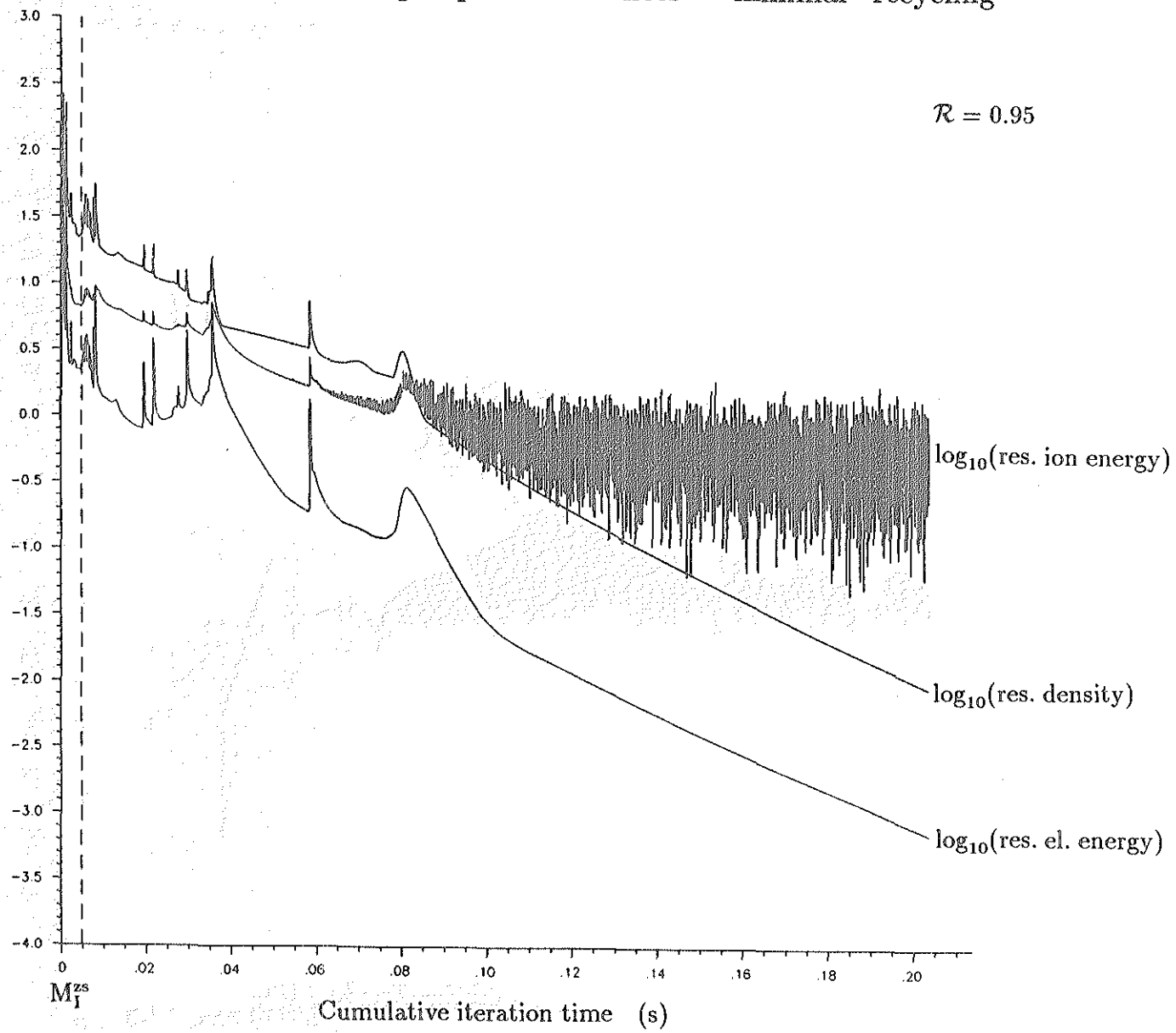


Fig.20 Decoupling of plasma balances – altered starting condition
– “minimal” recycling

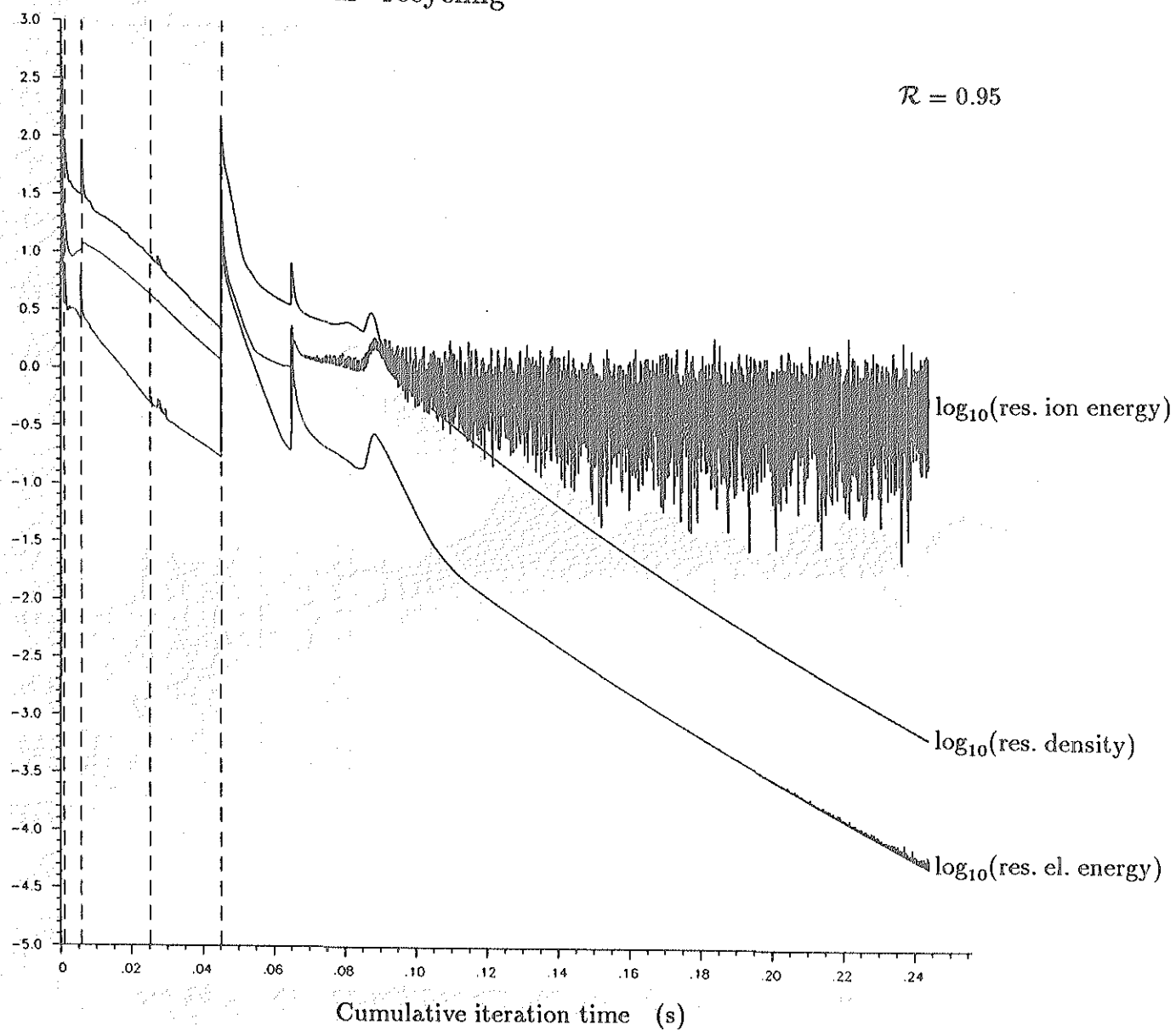


Fig.21 Stabilization for "1-D minimal" recycling
(atoms artificially constrained to magnetic surfaces)

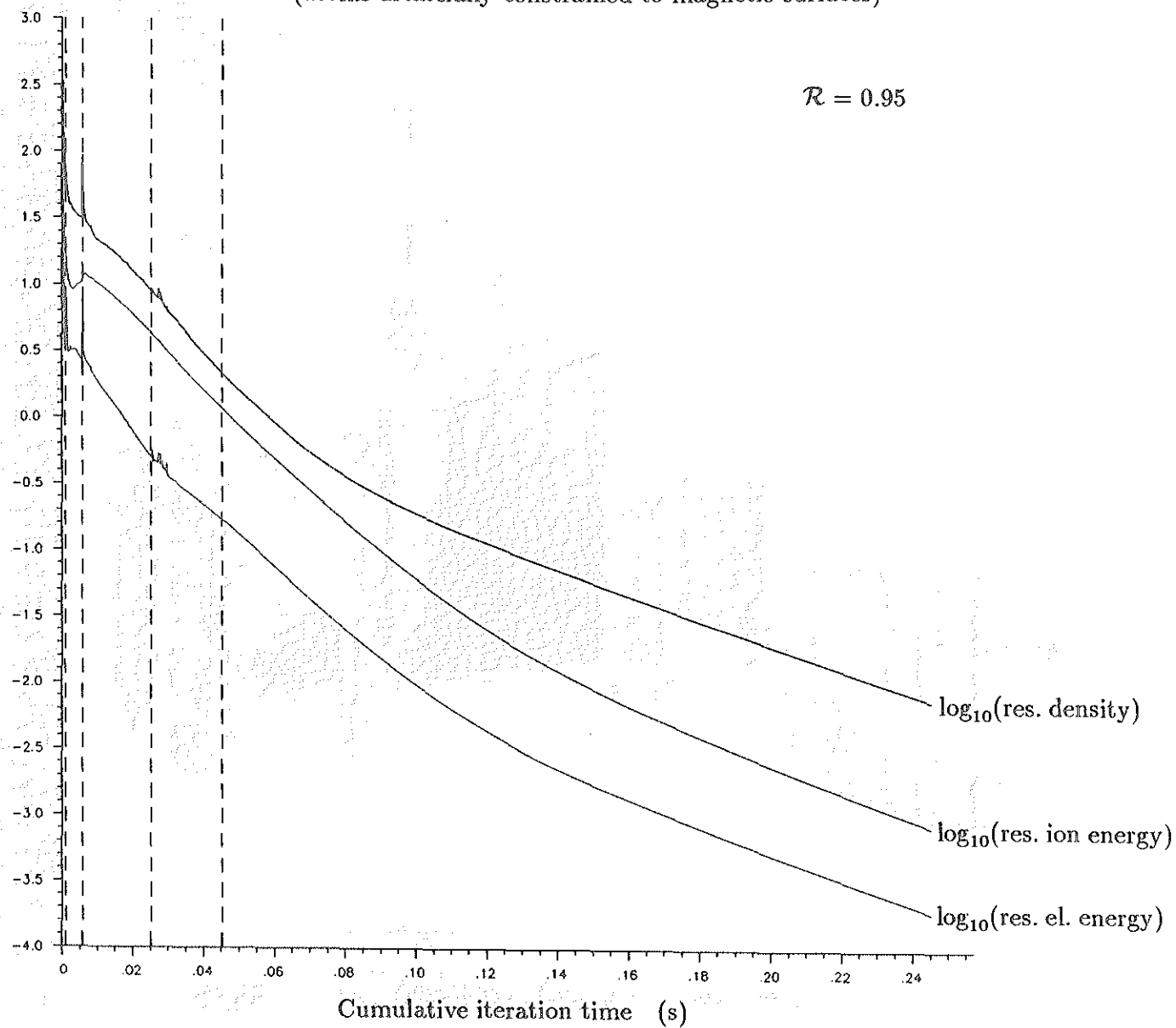


Fig.22 "B2"+EIRENE cycles – global balance errors
– removal of positive correlation
(continuation from Fig.6)

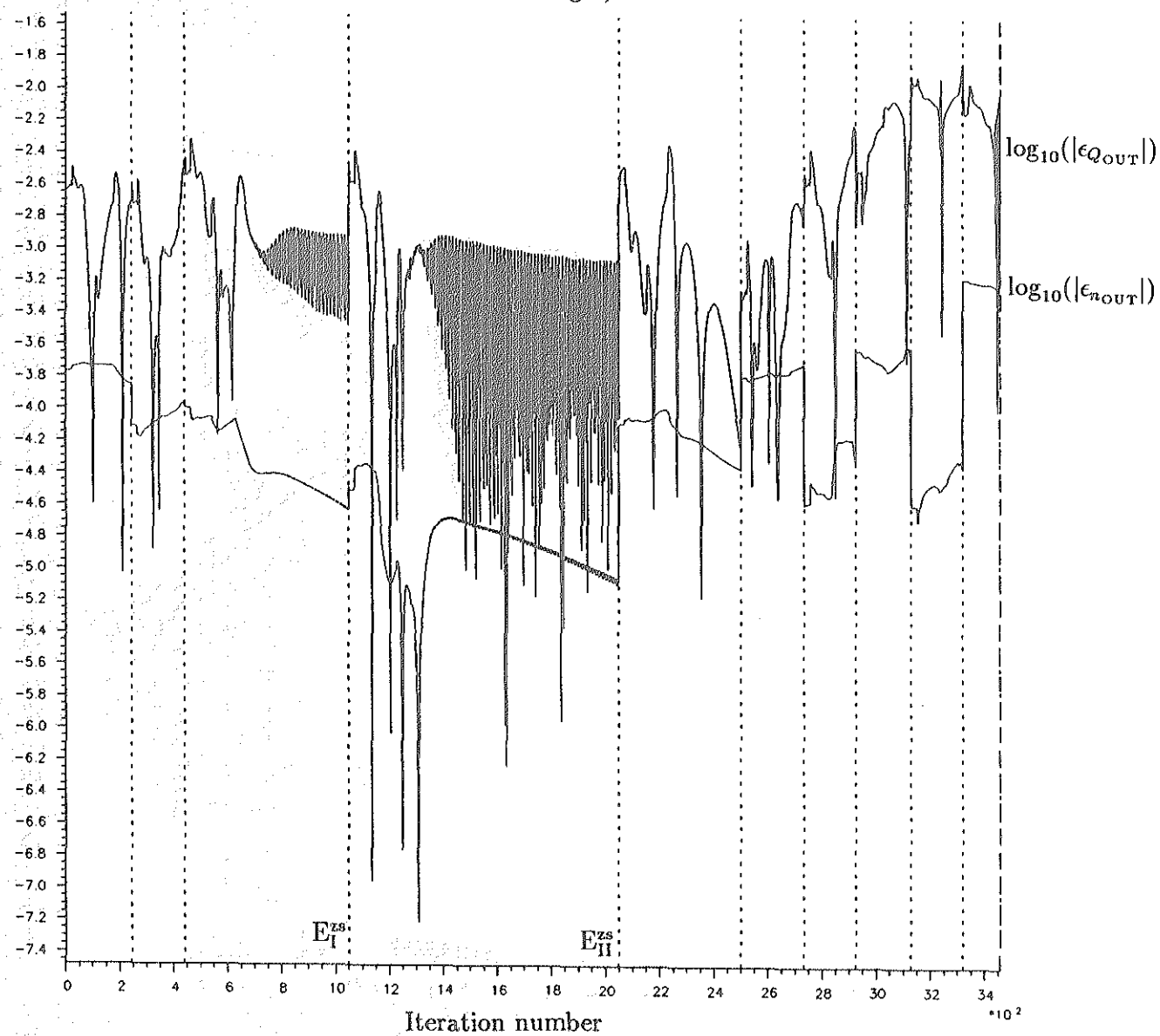
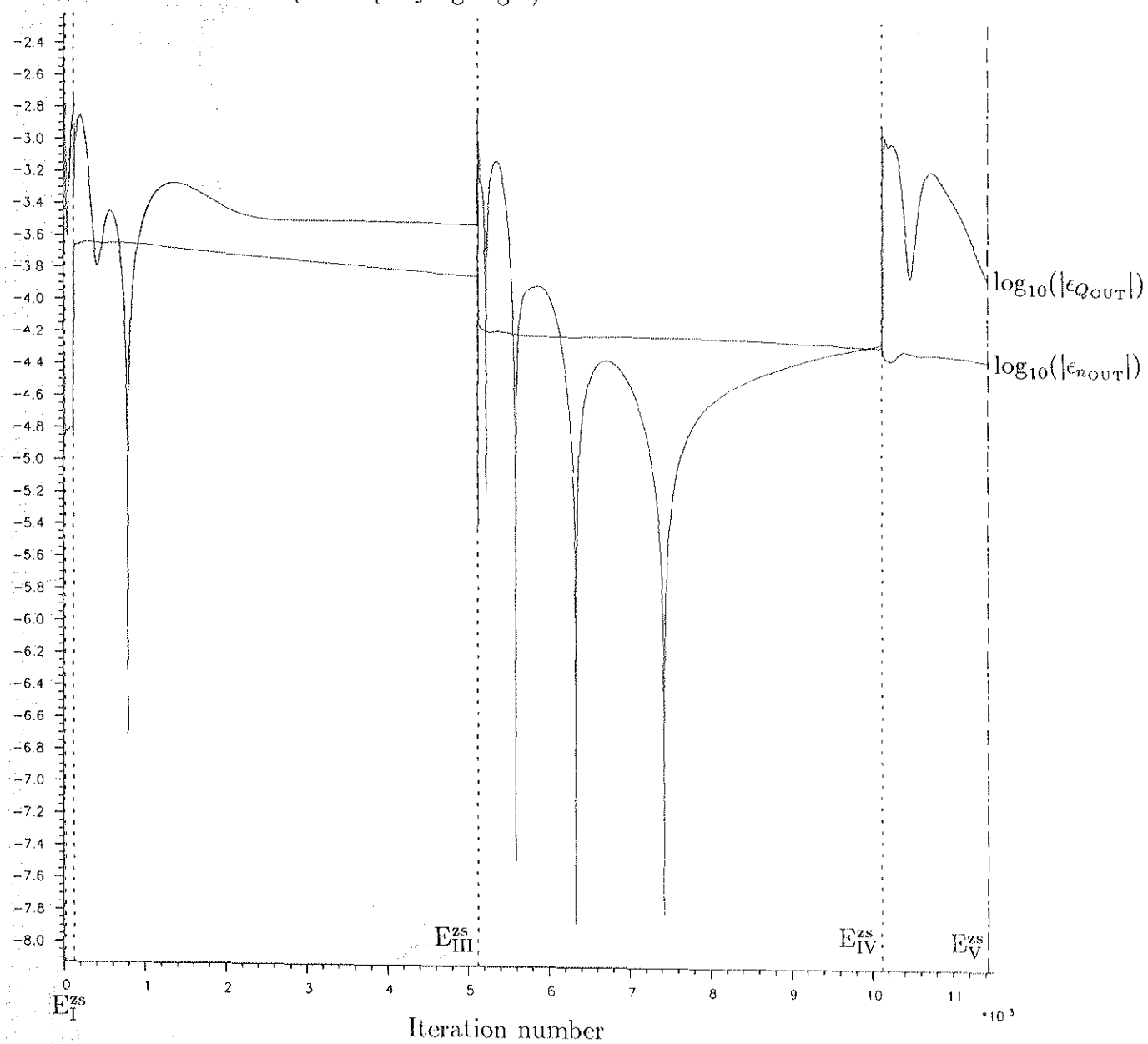
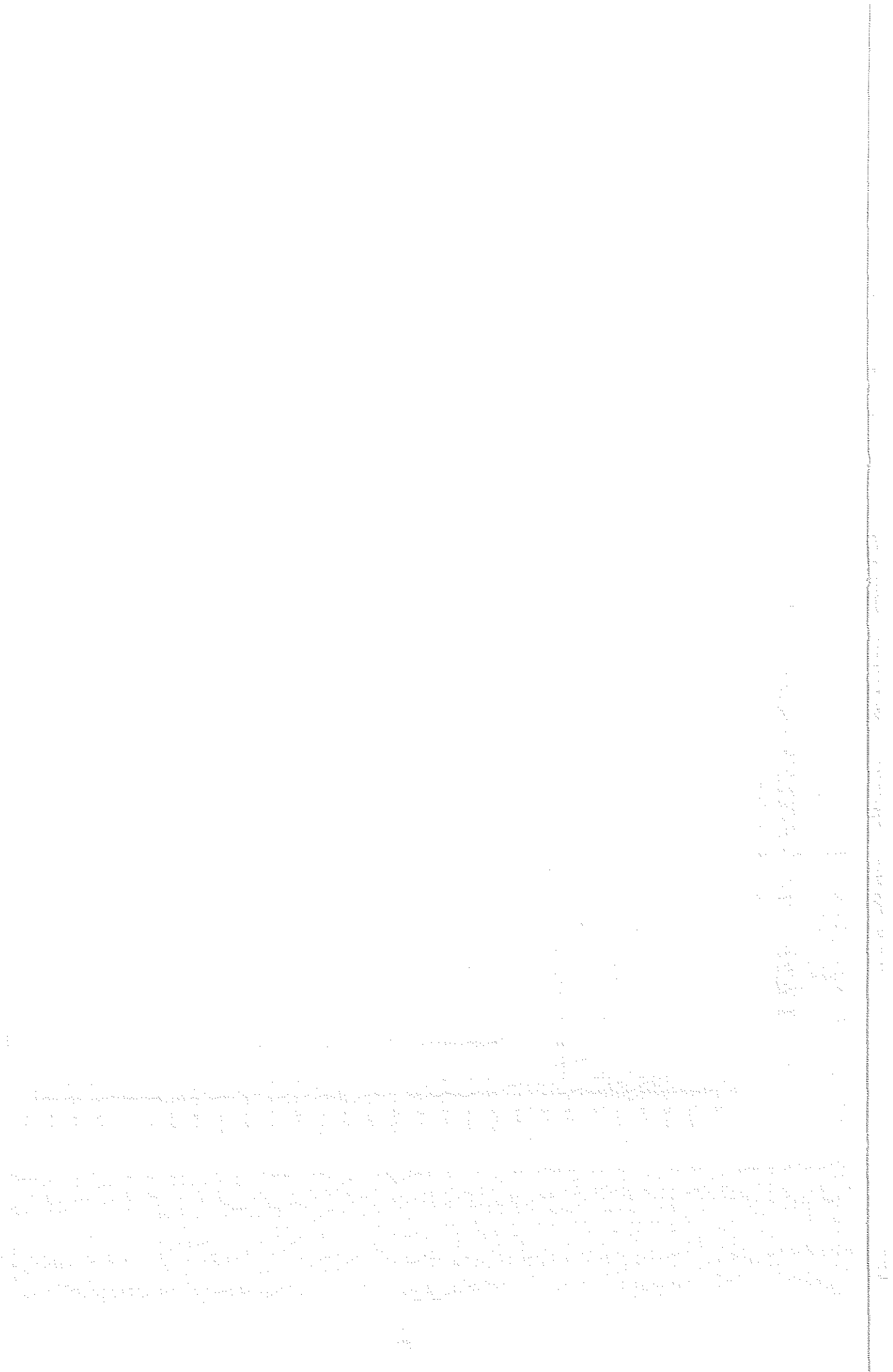


Fig.23 “B2”+EIRENE cycles – global balance errors
(accompanying Fig.3)





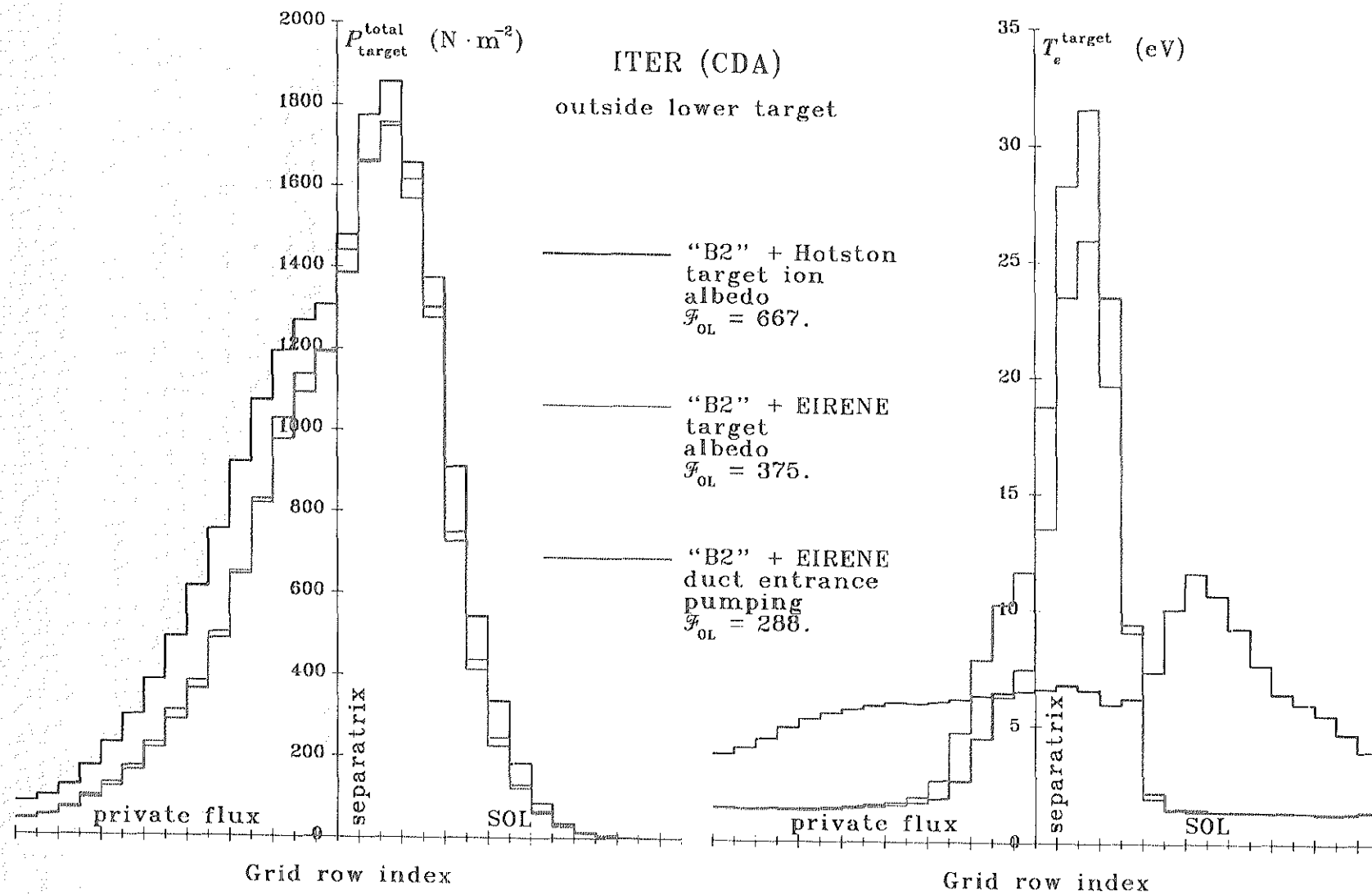


Fig.24

WALL

ITER (CDA)

"B2" + Hotston

target ion
albedo

$\mathcal{F} = 667.$

Local ion
flux Γ (s^{-1})
through each
cell

MID-PLANE

Magnitude ($10^{22} s^{-1}$)

-  > 3.5
-  $2.0 \rightarrow 3.5$
-  $0.5 \rightarrow 2.0$
-  < 0.5

CORE

PRIVATE FLUX

TARGET

π_i Braginskii

Fig.25

WALL

ITER (CDA)

"B2" + EIRENE

target
albedo

$\mathcal{F} = 375.$

Local ion
flux Γ (s^{-1})
through each
cell

MID-PLANE

Magnitude ($10^{22} s^{-1}$)

-  > 3.5
-  $2.0 \rightarrow 3.5$
-  $0.5 \rightarrow 2.0$
-  < 0.5

CORE

PRIVATE FLUX

TARGET

π_i Braginskii

Fig.25 contd...

WALL

ITER (CDA)

"B2" + EIRENE

duct entrance
pumping

$\mathcal{F} = 288.$

Local ion
flux Γ (s^{-1})
through each
cell

$\pi_i^{\parallel \parallel}$
Braginskii

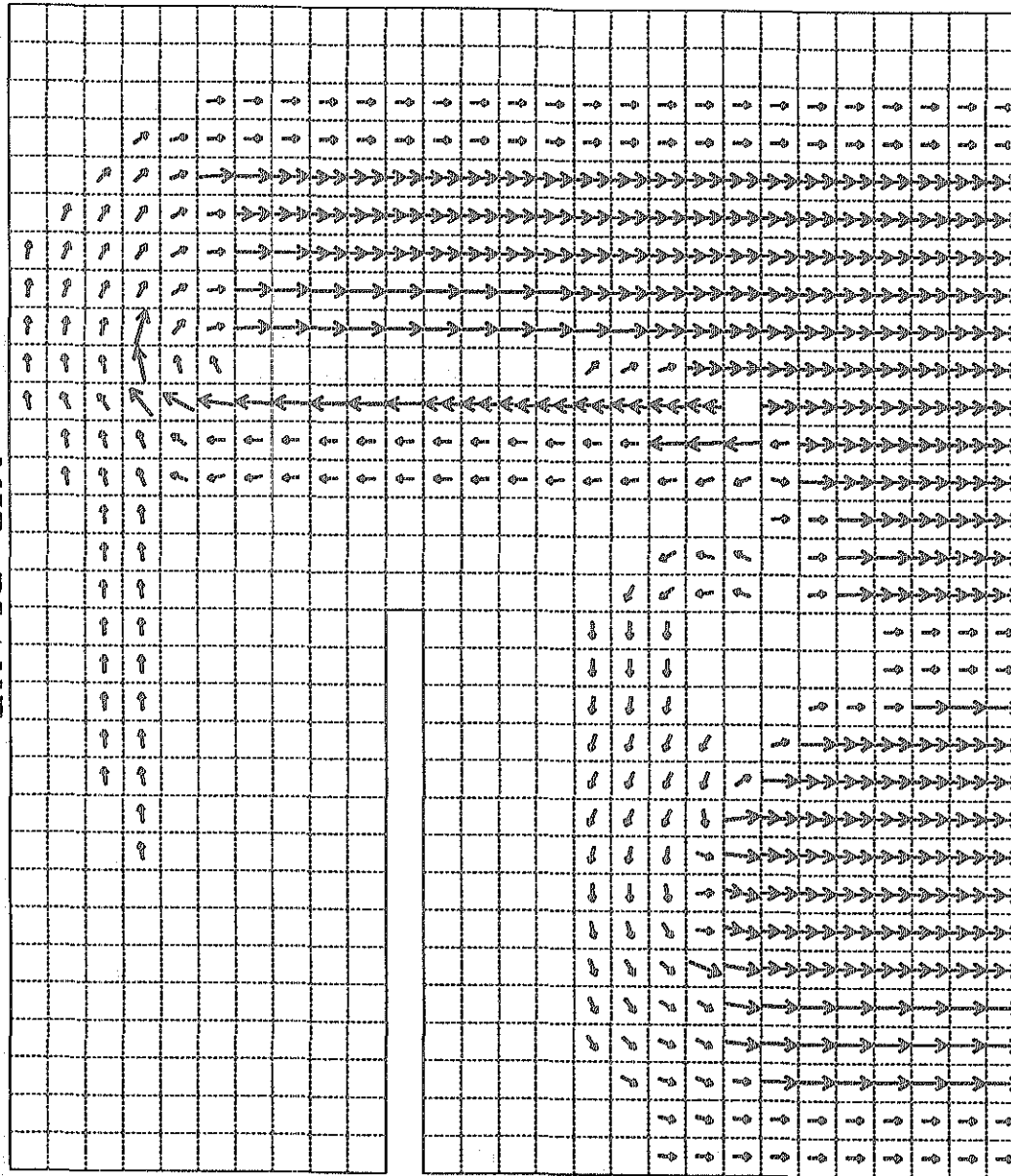
69

Magnitude ($10^{22} s^{-1}$)

-  > 3.5
-  $2.0 \rightarrow 3.5$
-  $0.5 \rightarrow 2.0$
-  < 0.5

MID-PLANE

TARGET

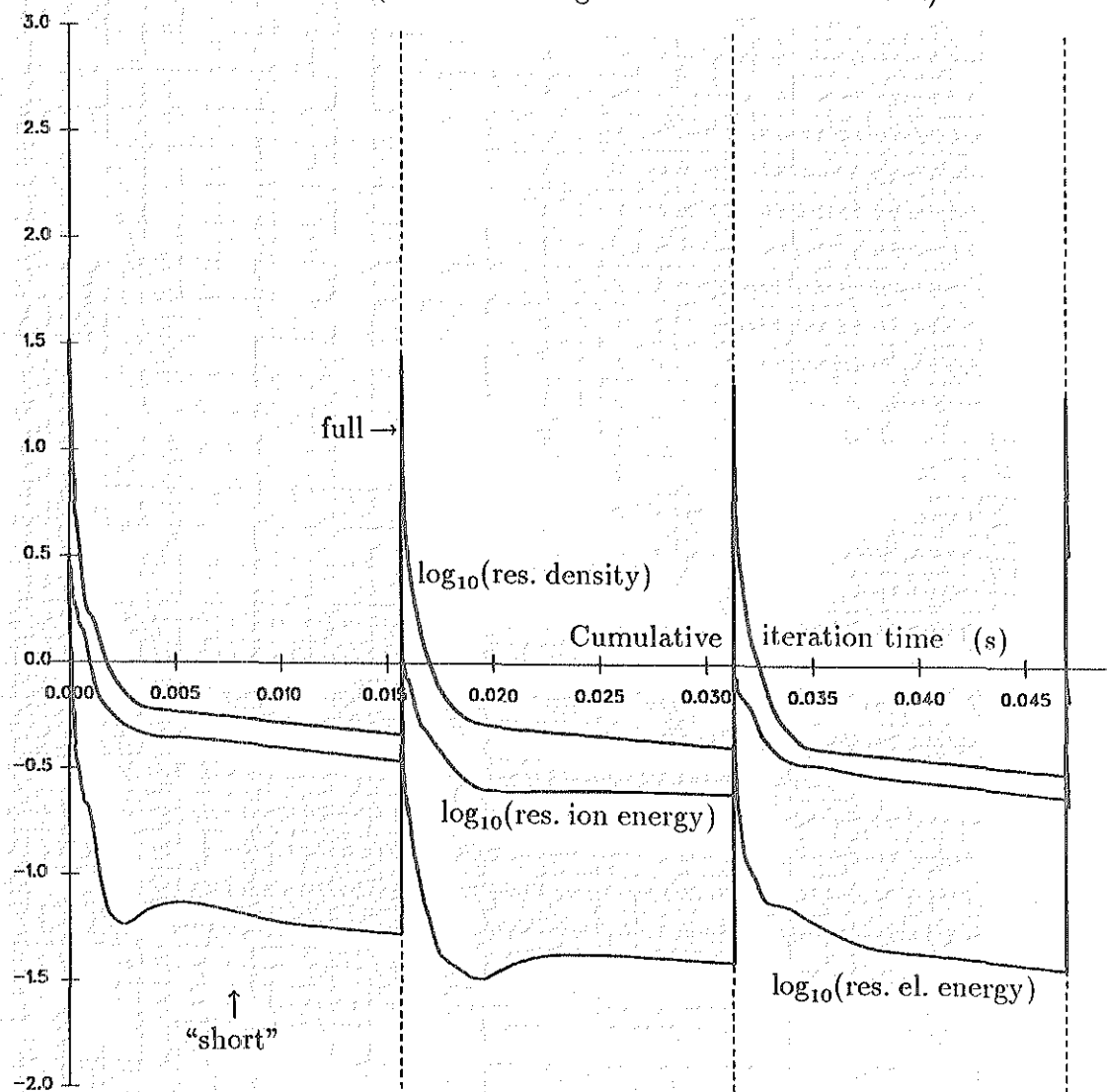


CORE

PRIVATE FLUX

Fig.25 contd...

Fig.26 Evolution of "B2"+EIRENE cycles -
Hotston-like target albedoes
(6×10^4 test-flights each Monte Carlo call)



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