An Algorithm for the Description of Impurity Diffusion under Finite Reaction Rates

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IPP 1/195 Oktober 1981

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in English

Abstract

An algorithm allowing a fast and stable solution of stationary and time dependent 1-d diffusion problems for the case of finite ionization and recombination rates is described. Test results of numerical computations and an analytic stability analysis show its unconditional stability for appropriate choice of the time-centering of the diffusion and possible drift terms. The computational effort rises linearly with the numbers of included ionization stages.

1. Introduction

The solution of the finite rate equations of impurity diffusion in a tokamak is of crucial importance both for the interpretation of experimentally observed distributions of impurity ion species in terms of transport models (e.g. /1/), and for a realistic assessment of the potential of radiating boundary layers as a means of energy transfer to the walls (see /2/ and references cited there). So far respective algorithms have proven usually to be too time-consuming to allow inclusion into general simulation codes and large-scale production runs. A limited number of full-scale discharge simulations, including the finite-rate effects, have recently been reported by Mercier et al. / 3 /.

Aiming at an interpretation of Pulsator /4/ and ASDEX /1/ impurity distribution measurements, Behringer and Engelhardt have been successful with using a relatively simple algorithm (called BE in the following) for the treatment of both the stationary and the time-dependent problem, which leads to a computational effort increasing only linearly with the number of ionic stages included in the computations. This was achieved by treating recombination only as perturbation term, computed explicitly from the results of the preceding iteration or time step. Intuition, test calculations, and the results of a stability analysis in section 4 show that this is indeed a valid method in cases dominated by diffusion and ionization, but has to run into numerical difficulties when approaching coronal equilibrium or other situations with important contributions from recombination.

This observation suggests a more symmetric treatment of ionization and recombination, which can be realized by alternating in successive steps between ionization and recombination as the terms treated explicitely or implicitely, respectively. The resulting algorithm (WL) conserves the advantageous scaling of the

computational effort with the number of included ionization stages, and has been shown unconditionally stable for all combinations of diffusion, ionization and recombination time constants. It is described, together with test calculations for simplified model systems, in section 2 as a solution method to the stationary, and in section 3 to the time-dependent problem. Section 4 describes the analytic stability analysis for the BE and WL algorithms, confirming the conclusions of the numerical tests.

2. Algorithm for the Stationary Problem

For outlining the algorithms and for the numerical tests described here we use a simple diagonal diffusion model with spatially constant coefficients and slab geometry. This should be a valid approach for testing stability properties; the additional complexities and couplings arising from additional (e.g. neoclassical) terms are discussed in section 5. The stationary system we then can write in matrix notation as

$$\overleftrightarrow{D}\,\frac{d^2}{dx^2}\,\vec{n} = \overleftrightarrow{S}\cdot\vec{n} + \overleftrightarrow{R}\cdot\vec{n} - \vec{d} \qquad (1)$$

with $\overleftrightarrow{D}$ a diagonal matrix and $\vec{n}$, $\overleftrightarrow{S}$, $\overleftrightarrow{R}$ and $\vec{d}$ vectors and matrices in the space of ionization stages

$$\vec{n} = \begin{bmatrix} n_1 \\ n_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ n_K \end{bmatrix} \qquad \overleftrightarrow{S} = \begin{bmatrix} s_1 & 0 & 0 & \cdot & \cdot & & \\ -s_1 & s_2 & 0 & \cdot & \cdot & & \\ 0 & -s_2 & s_3 & \cdot & \cdot & & \\ \cdot & \cdot & \cdot & \cdot & \cdot & & \\ & & & & & \cdot & \cdot \\ & & & & \cdot & s_{K-1} & 0 \\ & & & & 0 & -s_{K-1} & s_K \end{bmatrix} \qquad \overleftrightarrow{R} = \begin{bmatrix} r_1 & -r_2 & 0 & \cdot & & & \\ 0 & r_2 & -r_3 & \cdot & & & \\ 0 & 0 & r_3 & \cdot & & & \\ \cdot & \cdot & \cdot & & & & \\ & & & & \cdot & \cdot & \cdot \\ & & & & \cdot & r_{K-1} & -r_K \\ & & & & \cdot & 0 & r_K \end{bmatrix}$$

For simplicity we have absorbed here the electron density into the ionization and recombination rates s_j and r_j, respectively.

Using a diffusion-type model only for the ionized stages (n_j being j-times ionized), the ionization of neutral impurities is contained in the source term $\vec{d}$, which therefore has the form

$$\vec{d} = \begin{bmatrix} +d\ (x) \\ 0 \\ 0 \\ 0 \\ \cdot \\ \cdot \\ \cdot \\ 0 \end{bmatrix},$$

For the following we assume d(x) to be a given function (for the tests reported here, e.g. $d(x) = (\nu + 1) \cdot x^{\nu}$).

The algorithmic problem with eq.(1) is rather similar to that of a two-dimensional diffusion equation. Due to the structure of the $\overleftrightarrow{R}$ and $\overleftrightarrow{S}$ matrices, the ionization and recombination terms of the system look like a discrete analogon to a diffusion equation (with inhomogeneous coefficient) in the coordinate of the ionization state. Thus a host of numerical methods developed for 2-d elliptic problems could, in principle, be tested for their applicability. In particular, an alternating direction method based on treating ionization state and spatial variable as the two independent coordinates might be an alternative to the one described in the following.

Engelhardt /4/ has successfully applied the iteration scheme

$$\overleftrightarrow{D}\,\frac{d^2}{dx^2}\,\vec{n}^{\,\ell} - \overleftrightarrow{S}\,\vec{n}^{\,\ell} = \overleftrightarrow{R}\,\vec{n}^{\,\ell-1} - \vec{d} \qquad \text{(BE 1a), (WL 1a)}$$

where ℓ refers to the iteration cycle. Including at the

new level only ionization allows, due to the structure of the $\overleftrightarrow{S}$-matrix, to solve successively the diffusion equation for the ionization degrees in increasing order, using a standard algorithm for tri-diagonal matrices.

An extension to this, rendering the treatment symmetric in $\overleftrightarrow{R}$ and $\overleftrightarrow{S}$ consists in following each such step by another one of the form

$$\overleftrightarrow{D}\,\frac{d^2}{dx^2}\,\vec{n}^{\,\ell+1} - \overleftrightarrow{R}\,\vec{n}^{\,\ell+1} = \overleftrightarrow{S}\,\vec{n}^{\,\ell} - \vec{d} \qquad \text{(WL 1b)}$$

This modification conserves the advantage that again the equation for different ionization degrees can be solved one after the other, albeit here now in descending order.

Results of numerical tests of these two schemes are reported in figs. 1 and 2. The system tested corresponds to a simple model, with the absolute magnitude of all non-zero elements of the three matrices $\overleftrightarrow{D}$, $\overleftrightarrow{S}$, $\overleftrightarrow{R}$ equal to constants D_o, S_o, R_o, respectively. The character of the system then changes with the relative magnitudes of three time constants which are defined by

$$\tau_D = \left(D_o/(L)^2\right)^{-1},\ \tau_S = S_o^{-1} \quad \text{and} \quad \tau_R = R_o^{-1}$$

where L is the dimension of the system. Cases reported here correspond to ratios $\tau_D : \tau_S : \tau_R$ = (1:0.1:1), (1:1:0.1), (1:0.1:0.1), (1: 0.05:0.05), (1:0.01:0.01). The system used contained only four ionization stages; boundary conditions for the test were

$$\left.\begin{array}{l} \text{at } x=0: \dfrac{d}{dx}\,n_j = 0 \\ \text{at } x=L=1: \ n_j = 0 \end{array}\right\} \quad \text{for all ionization stages.}$$

Results given in figs. 1 and 2 show the rate of convergence of the two methods for the five different parameter combinations, in the form of log - log plots of the relative variation between two cycles (for each of the four variables) against the number of iterations. Whereas the method alternating in the implicit treatment of ionization and recombination was found to converge throughout (and even for more extreme parameter combinations like $(1:10^{-3}:10^{-3})$, the unidirectional BE method failed in the case (1:1:0.1) corresponding to dominating recombination rate, and when approaching coronal equilibrium situations $(1:10^{-2}:10^{-2})$.

3. Algorithm for the Time-Dependent Problem

Both for assistance in diagnostic interpretation of impurity injection experiments and as a potential component of 1-d simulation calculations, time-dependent calculations are of even greater practical importance. The system under otherwise identical assumptions to those of eq. (1) and using the same notation then reads

$$\frac{\partial}{\partial t}\vec{n} - \overleftrightarrow{D}\frac{\partial^2}{\partial x^2}\vec{n} = -\overleftrightarrow{S}\cdot\vec{n} - \overleftrightarrow{R}\cdot\vec{n} + \vec{d} \qquad (2)$$

Behringer and Engelhardt have used an algorithm including a Crank-Nicholson description of the diffusion term of the form

$$\frac{1}{\Delta t}\left(\vec{n}^{\ell} - \vec{n}^{\ell-1}\right) - \alpha\overleftrightarrow{D}\frac{\partial^2\vec{n}^{\ell}}{\partial x^2} + \overleftrightarrow{S}\vec{n}^{\ell} = (1-\alpha)\overleftrightarrow{D}\frac{\partial^2\vec{n}^{\ell-1}}{\partial x^2} - \overleftrightarrow{R}\vec{n}^{\ell-1} + \vec{d}^{\ell-\frac{1}{2}} \quad \text{(BE2), (WL 2a)}$$

with α the usual constant deciding the degree of time-centering of the spatial derivatives, and the index ℓ now referring to a time-step.

The corresponding "symmetrized" version consists in alternating such a time-step, with one of the form

$$\frac{1}{\Delta t}\left(\vec{n}^{\,\ell+1} - \vec{n}^{\,\ell}\right) - \alpha \overleftrightarrow{D} \frac{\partial^2 \vec{n}^{\,\ell+1}}{\partial x^2} + \overleftrightarrow{R}\,\vec{n}^{\,\ell+1} = (1-\alpha)\overleftrightarrow{D} \frac{\partial^2 \vec{n}^{\,\ell}}{\partial x^2} - \overleftrightarrow{S}\,\vec{n}^{\,\ell} + \vec{d}^{\,\ell+1/2} \qquad \text{(WL 2b)}$$

Again, by proceeding either up- or downwards the scale of ionization stages, the resulting difference equations can be solved by a usual routine for tri-diagonal systems.

Time-dependent test runs using the WL-algorithm, a value of $\alpha = 0.5$, $\Delta t = 10 \cdot (\Delta x)^2 / D_o$ and initial conditions $n_j(x) = 0$ were carried out for the otherwise same parameter combinations used in the time-independent runs of the previous section, with results illustrated in figs. 3a-e.
Shown are the temporal and spatial evolution of the 3rd ionization stage over the time interval $0 < t < 1$ and the region $0 < x < 1$. The diffusion constant D_o was kept constant, so that the changes in the ratios $\tau_D : \tau_S : \tau_R$ implied also variations in the ratio of time-step to ionization or recombination time. Consequently, in the most extreme case of fig. 3e, τ_S and τ_R were actually a factor three smaller than the time-step: of course, this does not correctly represent the initial dynamic, but the system remains stable and describes correctly the "quasi-coronal" development on the diffusive time scale.

To confirm the linear scaling of operations with the number of species treated, to obtain quantitative information about the required computation time, and to get a preliminary idea about the importance of round-off errors, comparison runs were made over 500 time-steps with 48 grid points, for systems with 4, 8 and 16 ionization stages, in single precision using the IPP Amdahl VM/470 and with the doubled precision on our CRAY.

The results for the required computer time per time step are given in table 1. Of course, due to the simplicity in the chosen system, no computation time was required for setting up the $\overleftrightarrow{D}$, $\overleftrightarrow{R}$ and $\overleftrightarrow{S}$ matrices, so that the numbers in table 1 are only of indicative value.

TABLE 1

computer time per time step for system with 48 spatial grid points

number of ionization stages treated: n_K	AMDAHL VM/470 [sec]	CRAY [sec]
4	6×10^{-3}	1.4×10^{-3}
8	8.8×10^{-3}	1.8×10^{-3}
16	1.4×10^{-2}	2.6×10^{-3}

The actually even less than linear increase with n_K is of course a consequence of the better amortization of the overhead operations. Comparison of Amdahl and Cray results also showed that round-off errors are still not important for this system even when using single precision: the relative deviation between results for the 16^{th} ionization stage for the case $\tau_D : \tau_S : \tau_R = 1 : 10^{-2} : 10^{-2}$ was less than 2×10^{-4}.

4. Analytic stability analysis for the time dependent algorithm

The favourable stability properties of the scheme described by the equations WL2a + WL2b can also be ascertained by an amplification factor analysis like outlined e.g. in Ref. / 5 /. The only non-standard part of it consists in a Fourier decomposition of the errors $\delta \vec{n}$ also with regard to the ionization stage, writing

$$\delta n_j^{\ell-1}(x) = \sum_{m=0}^{\infty} \sum_{k=1}^{K} N_{m,k}\, e^{i\pi k \frac{j}{K}}\, e^{i\pi m \frac{x}{L}} .$$

The amplification factor of the step WL2a (= BE2) for the m, k error component $N_{m,k}$ can then be computed as

$$\gamma_{BE} = \frac{1 + (1-\alpha)c - 2\left(\sin\pi\frac{k}{2K}\right)^2 R_o \Delta t + 2i R_o \Delta t \cdot \sin\pi\frac{k}{2K} \cdot \cos\pi\frac{k}{2K}}{1 - \alpha c + 2\left(\sin\pi\frac{k}{2K}\right)^2 S_o \Delta t + 2i S_o \Delta t \cdot \sin\pi\frac{k}{2K} \cdot \cos\pi\frac{k}{2K}} \qquad (3)$$

with c as an abbreviation of the term

$$c = 2\left(\cos\left(\pi m\frac{\Delta x}{L}\right) - 1\right) \cdot D_o \frac{\Delta t}{(\Delta x)^2} \qquad (4)$$

known from the analysis of the Crank Nicholson scheme. For error damping in this simple repeated algorithm (the BE scheme), we require

$$\gamma_{BE}\,\gamma^{*}_{BE} = \frac{(1+(1-\alpha)c)^2 - 4\left(1+(1-\alpha)c\right)R_o\Delta t\left(\sin\pi\frac{k}{2K}\right)^2 + 4(\Delta t)^2 R_o^2\left(\sin\pi\frac{k}{2K}\right)^2}{(1-\alpha c)^2 + 4(1-\alpha c)\cdot S_o\Delta t\left(\sin\pi\frac{k}{2K}\right)^2 + 4(\Delta t)^2 S_o^2\left(\sin\pi\frac{k}{2K}\right)^2} < 1$$

over the whole range of

$$-2 < \cos\left(\pi m\frac{\Delta x}{L}\right) - 1 < 0$$

$$0 < \sin^2\left(\pi\frac{k}{K}\right) < 1$$

which for arbitrary values of Δt is the case only for $R_o < S_o$ and $\alpha \gtrsim 0.5$

For the symmetrized, two step algorithm (WL scheme) the amplification factor over a whole cycle reads

$$\gamma_{WL} = \frac{\eta_1^2 - 2\left(\eta_1\Delta t\,(R_o+S_o) - 2(\Delta t)^2 R_o S_o\right)\left(\sin\pi\frac{k}{2K}\right)^2 + 2i\,\eta_1\Delta t\,(R_o - S_o)\cdot\sin\pi\frac{k}{2K}\cdot\cos\pi\frac{k}{2K}}{\eta_2^2 + 2\left(\eta_2\Delta t\,(R_o+S_o) + 2(\Delta t)^2 R_o S_o\right)\left(\sin\pi\frac{k}{2K}\right)^2 - 2i\,\eta_2\Delta t\,(R_o - S_o)\cdot\sin\pi\frac{k}{2K}\cdot\cos\pi\frac{k}{2K}} \qquad (5)$$

with the abbreviations

$$\eta_1 = 1 + (1-\alpha)c$$

$$\eta_2 = 1 - \alpha c$$

As $\eta_2 > 0$ and $|\eta_1| < |\eta_2|$, from this expression follows stability for $\alpha \gtrsim 0.5$ for all values of Δt and independently of the relative magnitudes of R_o and S_o.

5. Extension to more general systems

Both numerical tests and a formal stability analysis have therefor shown at least for the somewhat idealized set of equations unconditional stability of the proposed WL algorithm, which because of its structure allows for a very fast solution. The general system of equations describing impurity diffusion in tokamaks contains additional terms which by altering the structure of the system could influence the stability properties of the method and - by providing additional coupling - its favourable scaling with the number of ion stages included. The additional terms ("anomalous" pinch terms, temperature gradient and proton density gradient term) not conserving the structure of equ. (2) are of the form

$$\overleftrightarrow{v}\,\frac{\partial}{\partial x}\,\vec{n}$$

In the pure diffusion equation (neglecting ionization and recombination) such terms, if discretized by

$$v\frac{\partial}{\partial x}n \approx v\cdot\left(n^{\ell,i+1} - n^{\ell,i-1}\right)\frac{\alpha}{2\Delta x} + v\cdot\left(n^{\ell-1,i+1} - n^{\ell-1,i-1}\right)\cdot\frac{1}{2\Delta x}(1-\alpha)$$

modify the amplification factor from

$$g = \frac{1 + c(1-\alpha)}{1 - c\alpha}$$

to

$$\sqrt{g\,g^*} = \frac{\left(1 + c(1-\alpha)\right)^2 + \beta^2(1-\alpha)^2}{(1-c\alpha)^2 + \beta^2\alpha}$$

with

$$c = 2\left(\cos\left(\pi m \frac{\Delta x}{L}\right) - 1\right)$$

$$\beta = v \cdot \sin\left(\pi m \frac{\Delta x}{L}\right) \cdot \frac{\Delta t}{\Delta x} ,$$

and conserve therefore the unconditional stability for $\alpha \gtrsim 0.5$.

A formal stability analysis of the complete system, including drift terms, has not been carried out, but fairly extensive numerical tests found also in this case no instabilities when using the WL-algorithm for ionization and recombination terms and a Crank-Nicholson parameter in the range $0.5 \lesssim \alpha < 1$.

Terms complicating the sequence of calculations are the neoclassical contributions to transport arising from collisions of ionic species n_j with impurity particles in a different ionization stage. Such terms, which constitute a generally weak nonlinearity, should conveniently be treated by a description of the interaction as between the test species n_j and an appropriate "average" background ion.

In addition to the above tests for "idealized" systems in slab geometry with constant ionization and recombination rates, calculations have been carried out also for realistic cases in cylindrical geometry, using measured temperature and density profiles and available information on the ionization and recombination rates of oxygen and iron. Results of these further studies which will be published in another report confirmed the favourable stability behaviour of the WL-algorithm and clarified the resulting relation between time step size and resolution requirements in the realistic multi-timescale system.

Acknowledgement

The authors are grateful to Dr. W. Schneider for carrying out comparison calculations with a code created by his program generator "DEQTRAN" /6/.

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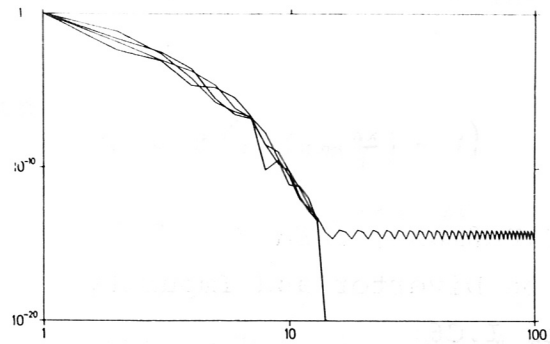
Figure Captions

Fig. 1 Convergence rates of the (BE)-algorithm for stationary ionization state distribution, for various ratios $\tau_D : \tau_S : \tau_R$. Shown are the relative variation between results of two successive iteration cycles as a function of iteration number, for all 4 ionization stages of the test system.

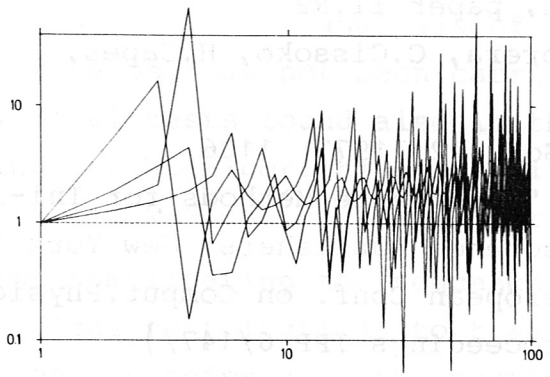
Fig. 2 Results of the WL algorithm for the cases of Fig. 1.

Fig. 3 Results of time-dependent calculations with the WL algorithm for otherwise same parameters combinations as used in Fig. 1 and 2. Shown is the time-evolution of the spatial distribution of the 3rd (of four) ionization stages included.



$\tau_D : \tau_S : \tau_R$

1 : 0.1 : 1



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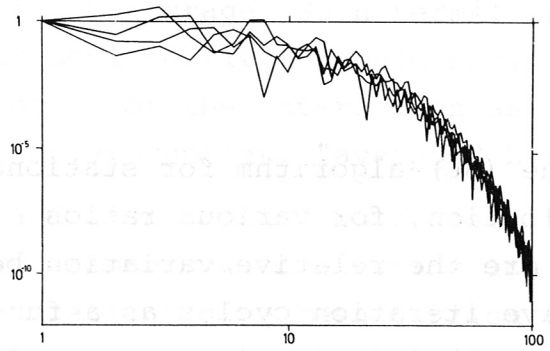

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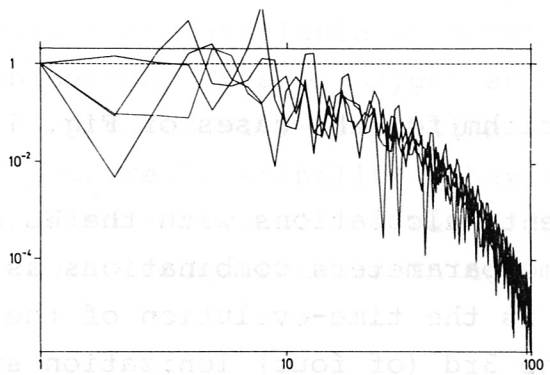

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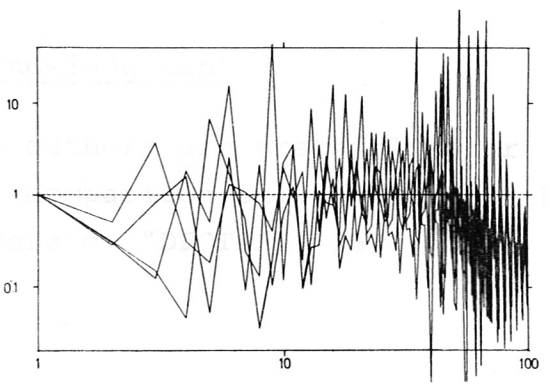

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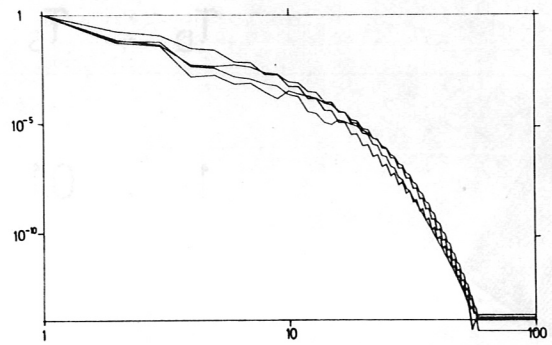
Fig. 1



τ_D : τ_S : τ_R

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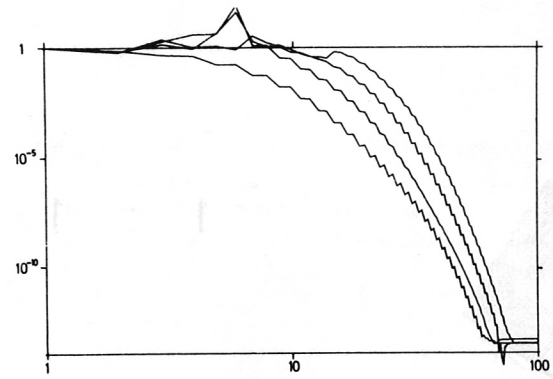

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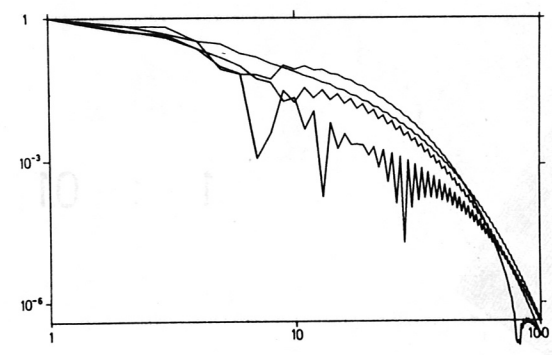

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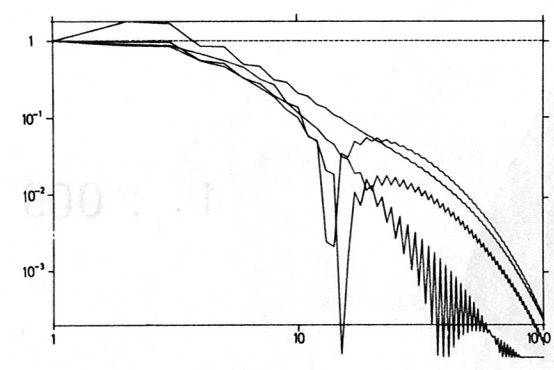

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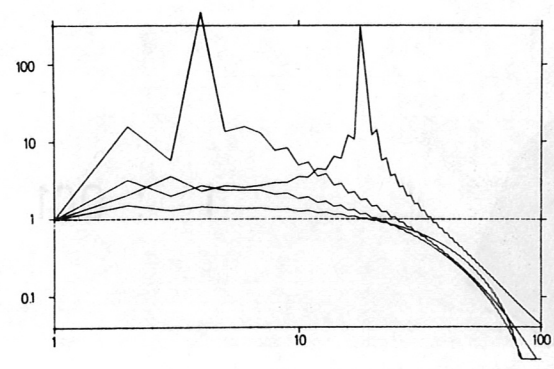

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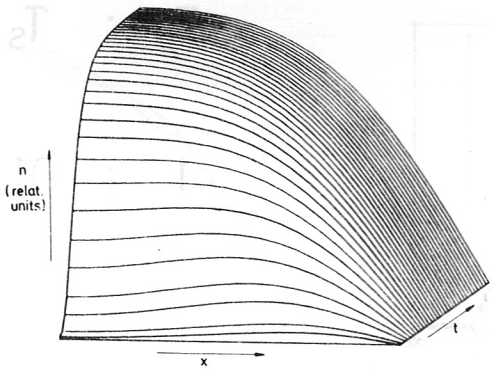
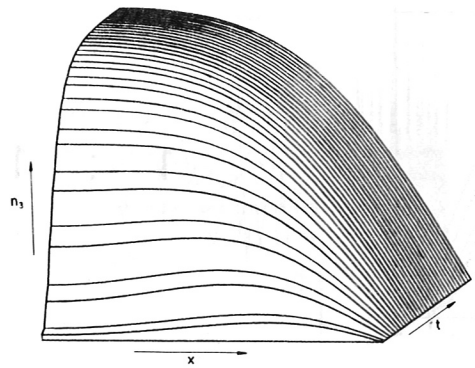
Fig. 2



$\tau_D : \tau_S : \tau_R$

1 : 0.1 : 1



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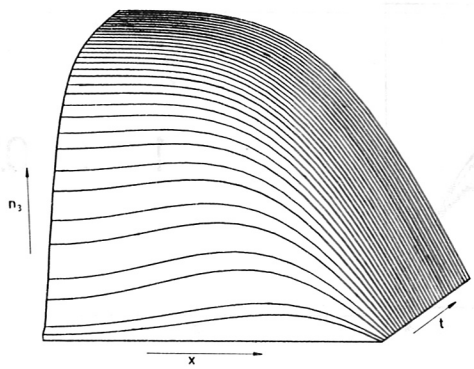

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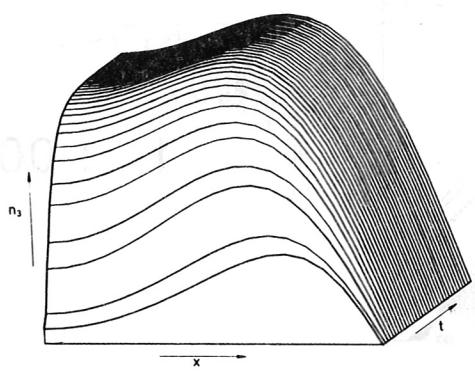

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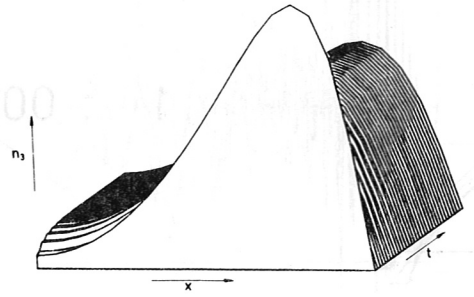

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Fig. 3