A discussion on

The Semi-implicit Formulation Of The Radial Impurity Transport Equation for tokamak plasmas &

Its application for estimating the fluctuation induced transport at the edge regions of the **ADITYA tokamak in India**

by

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Presented to:

The Princeton Plasma Physics Laboratory – ITER & Tokamak

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A bit about me...

2009 - B.Sc. (Physics, Lady Brabourne College, University of Calcutta, India)

- 2012 M.Tech. (Nuclear Science & Engineering, Department of Physics & Astrophysics, **University of Delhi, India)**
- 2019 Ph.D. (Nuclear Engineering & Technology Programme, Indian Institute of Technology **(IIT) Kanpur, India)**; Submitted thesis in 2019, Defended in July 2020

Ph.D. thesis title:

A novel approach towards solution of the radial impurity transport equation in tokamak plasma with a semi-implicit numerical method and an estimation of impurity transport in the Aditya tokamak

Ph.D. thesis supervisors:

Prof. Prabhat Munshi, Department of Mechanical Engineering, IIT Kanpur, India Prof. Joydeep Ghosh, Aditya–U tokamak, Institute for Plasma Research (IPR) Gandhinagar, India



Faculty Building, IIT Kanpur

(image courtesy: https://en.wikipedia.org/wiki/File:IIT Kanpur Faculty Building.JPG



Main Building, IPR Gandhinagar (image courtesy: http://www.ipr.res.in/HPRFM2013/documents/venue.html

Currently in India it is 23:00 hrs (11:00 PM IST) !

Time difference between IST & ET (USA): <u>9.5 hours</u>...

Outline

- 1. A brief overview on the 'Impurities' in tokamaks
- 2. The Aditya tokamak in India
- 3. The Radial Impurity Transport Equation (RITE)
- 4. A Semi–implicit numerical method for solving the RITE
- 5. The von Neumann stability analysis of the linearized Semi-implicit formulation of the RITE
- 6. Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma
- 7. Conclusions and Acknowledgements

A brief overview on the 'Impurities' in tokamaks

- Plasma impurities ^[1]: Non–fuel elements within plasma; never completely mitigated – affect tokamak operations; amount must be controlled
- Impurities: 'INTRINSIC' (inherently present) or 'EXTERNALLY INJECTED'; Intrinsic impurities (C, Fe, Mo, W) generate from Plasma Facing Components (PFCs)
- **PFC impurities:** caused by physical/chemical sputtering; large incoming of particle & thermal flux on PFCs/chemical reaction (hydrogen and carbon)
- Oxygen (O) enters through vacuum system walls; cause oxidation of hydrogen isotope (H₂O) and other impurity elements
- High impurity neutral concentration near edge; gradually enter the core:
 - ✓ Medium Z (Fe)/ High Z (Mo, W) impurities retain orbital electrons at higher T_e; cause plasma dilution and radiation throughout (mostly core)
 - \checkmark Low Z (Li, Be, B, C, N, O, Ne) impurities fully devoid of orbital electrons at T_e < 1 keV; ions confined towards edge for core $T_{e} \sim in \text{ keV}$; edge plasma radiation
 - **Collisions with electrons and ions (main & impurity)** characteristic ion radiations based on \checkmark collision phenomena (excitation: ionization, recombination, charge exchange)

[1] Wesson, J., *Tokamaks*, 3rd Edition, Clarendon Press, Oxford, 2004

The Aditya tokamak in India

The Aditya tokamak^[2]: Medium sized; Plasma enclosed in circular graphite limiter

• Aditya parameters:

- ✓ Major radius $R_0 = 0.75$ m; Minor radius $r_0 =$ 0.25 m
- ✓ Max. central toroidal field $B_{t.o} = 1.2$ T; Total toroidal field coils = 20
- ✓ For experiments and regular studies:
 - \blacktriangleright Central toroidal field B_{t. o} = 0.75 T
 - Plasma discharge duration ~ 100 ms
 - Plasma current: 80 100 kA
 - ➢ 28GHz; 200KW Electron cyclotron resonance heating (ECRH) system
 - \geq 20 40 MHz; 200 KW Ion cyclotron resonance heating (ICRH) system
 - Neutral gas entered: pre-fill or gas-puff system

Aditya now upgraded to Aditya-U tokamak

[2] Tanna, R. L., Ghosh, J., Chattopadhyay, P. K., Raj, H., Patel, S., Dhyani, P., Gupta, C. N., Jadeja, K. A., Patel, K. M., Bhatt, S. B., et al., 'Overview of recent experimental results from the Aditya tokamak', Nuclear Fusion, 57, 102008, 2017







The Radial Impurity Transport Equation (RITE) for the tokamak plasma

The Governing Equation

The RITE equation^[3] for each ionization state Z: non–linear, second–order in space, first-order in time, parabolic partial differential equation

$$\frac{\partial n_z(r,t)}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} r \left(D(r) \frac{\partial n_z(r,t)}{\partial r} - v(r) \right)$$

The **REACTION** term **S**_n, **(r,t)** leads to a <u>coupled</u>, <u>non–linear</u> PDE for each Z

$$S_{nz}(r,t) = \begin{cases} n_e(r) n_{z-1}(r,t) S_{z-1}(r) - r \\ n_e(r) n_{z+1}(r,t) \alpha_{z+1}(r) - n \\ \hline n_{i0}(r) n_{z+1}(r,t) \alpha_{z+1}^{cx}(r) - n \end{cases}$$

 $n_{z-1}(r,t)$, $n_z(r,t)$, $n_{z+1}(r,t)$: Impurity ion number density (m⁻³) for charge states Z-1, Z, and Z+1 $n_e(r)$: Electron number density (m⁻³) $n_{i0}(r)$: Neutral hydrogen (or H –isotope) number density (m⁻³) [3] TFR Group, 'Light impurity transport in TFR tokamak: Comparison of oxygen and carbon line emission with

 $(r, t) + S_{nz}(r, t) + S_{nz}(r, t) \text{ where, } Z = 1, 2, 3....N$

 $n_{i0}(r) n_z(r,t) \alpha_z^{CX}(r)$ CHARGE EXCHANGE (7 7+1)

 $n_{e}(r) n_{z}(r,t) S_{z}(r) + in_{e}(r) n_{z}(r,t) \alpha_{z}(r) + in_{e}(r) n_{z}(r) + in_{e}(r) + in_$ **IONIZATION (Z-1, Z)** (Z, Z+1)

numerical simulations', *Nuclear Fusion*, 22(9), pp. 1173–1189, 1982

What is being done actually?



A Semi-implicit numerical method for solving the RITE (1/10)

RITE^[4]: A form of Diffusion–Convection–Reaction equation

Non-conservative formulation of the transport equation

 $\frac{\partial n_{z}(r,t)}{\partial t} = \begin{cases} D(r)\frac{\partial^{2}n_{z}(r,t)}{\partial r^{2}} + \frac{\partial D(r)}{\partial r}\frac{\partial n_{z}(r)}{\partial r} \\ v(r)\frac{\partial n_{z}(r,t)}{\partial r} - n_{z}(r,t)\frac{\partial v(r)}{\partial r} - dr \end{cases}$

D(r) : Magnetic flux s

v(r) : Magnetic flux surface averaged convective velocity due to particle drifts S_{nz} (r, t) : Magnetic flux surface averaged cumulative REACTION term



[4] Sudo, S., Tamura, N., Funaba, H., Muto, S., Suzuki, C., Murakami, I., 'Impurity transport study with TESPEL injection and simulation', Plasma and Fusion Research: Regular articles, 8, 2402059, 2013

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$$\frac{(r,t)}{r} + \frac{D(r)}{r} \frac{\partial n_{z}(r,t)}{\partial r} - \begin{cases} \frac{v(r)}{r} & n_{z}(r,t) + S_{nz}(r,t) \end{cases} \\ \frac{v(r)}{r} & n_{z}(r,t) + S_{nz}(r,t) \end{cases}$$
(Z = 1, 2, 3....N)

Coefficients

$$= 0, \text{ for all } 0 \le r \le r_{o}$$

$$\implies \frac{dn_{z}}{dr}\Big|_{r=r_{o}} = -\frac{n_{z}}{l_{d}}, \text{ for all } 0 \le t \le t_{s}$$

$$\implies \frac{dn_{z}}{dr}\Big|_{r=0} = 0, \text{ for all } 0 \le t \le t_{s}$$

$$\xrightarrow{(t_{s}: \text{ Time to attain steady-attain steady-state)}}$$

A Semi-implicit numerical method for solving the RITE (2/10)

Earlier numerical schemes for solving the RITE

- Two separate time treatment of the constituent terms of RITE (Lackner et al.; Behringer et al.)- Numerical scheme in existing impurity transport code STRAHL
 - **Diffusion & convection terms** treated in time with implicit **Crank–Nicholson method** \checkmark
 - ✓ Ionization & recombination terms rendered implicit or explicit alternatively in consecutive time iterations
- Numerical scheme for the non-conservative formulation of the radial impurity transport equation (RITE) in **STRAHL^{[5],*}** code:

(jth iteration) $\frac{n^{j+1} - n^j}{\Delta t} = \widehat{D} \frac{\partial^2 n^{j+1/2}}{\partial r^2} + \left(\frac{\widehat{D}}{r} + \frac{d\widehat{D}}{dr} - \widehat{v}\right) \frac{\partial n^{j+1/2}}{\partial r} - \left(\frac{\widehat{v}}{r} + \frac{d\widehat{v}}{dr}\right) n^{j+1/2} - \widehat{S} n^{j+1} - \widehat{R} n^j + \widehat{d}$ (j+1th iteration) $\frac{-n^{j}}{dt} = \widehat{D}\frac{\partial^{2}n^{j+1/2}}{\partial r^{2}} + \left(\frac{\widehat{D}}{r} + \frac{d\widehat{D}}{dr} - \widehat{v}\right)\frac{\partial n^{j+1/2}}{\partial r} - \left(\frac{\widehat{v}}{r} + \frac{d\widehat{v}}{dr}\right)n^{j+1/2} - \widehat{S}n^{j} - \widehat{R}n^{j+1} + \widehat{d}$

Absence of stability analysis with all constituent terms of RITE in STRAHL, coordinate transformation from radial to the generalized magnetic flux surface coordinates, as reported ^[5], must take care that Δr remains below ± 10%

[5] Dux, R., 'Impurity Transport in tokamak plasma' – STRAHL manual, IPP 10/27 Garching, 2005

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A Semi-implicit numerical method for solving the RITE (3/10)

Earlier numerical schemes for solving the RITE

- Behringer et al.^[6]: central-difference scheme in space (r); time-centred Crank-Nicholson scheme
- Assumption in model: transport coefficients spatially constant; solutions determined for slab geometry
- Time-centred Crank-Nicholson method: Shortcomings upon expressing impurity number densities (n_{z}) in previous (j-1) and current (j) time iterations
- Set of equations solved for $Z = 1 \rightarrow N$ (ascending), term $n_{z+1, j+1}$ ($n_e n_{z+1} \alpha_{z+1}$) then unknown; for $Z = N \rightarrow 1$ (descending), term $n_{z-1, j+1}$ ($n_e n_{z-1} S_{z-1}$) then unknown

$$\frac{n^{j+1} - n^j}{\Delta t} = \widehat{D} \frac{\partial^2 n^{j+1/2}}{\partial r^2} + \left(\frac{\widehat{D}}{r} + \frac{d\widehat{D}}{dr} - \widehat{v}\right) \frac{\partial n^{j+1/2}}{\partial r}$$
where, $n_z^{j+\frac{1}{2}} = \frac{n_z^{j+1} + n_z^j}{2}$ (Analogous)

[6] Behringer, K., 'Description of impurity transport code STRAHL', JET-R (87) 08, Report, JET Joint Undertaking, Culham, 1987

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 $\frac{\sqrt{2}}{r} - \left(\frac{\hat{v}}{r} + \frac{d\hat{v}}{dr}\right) n^{j+1/2} - \hat{S} n^{j+1/2} - \hat{R} n^{j+1/2} + \hat{d}$

s expressions for \mathbf{n}_{z-1} and \mathbf{n}_{z+1} ; Z= 1, 2, 3... N)

A Semi-implicit numerical method for solving the RITE (4/10)

Earlier numerical schemes for solving the RITE

- Alternation of ascending and descending Z in consecutive time cycles:
 - ✓ **Recombination** term calculated in **1**st cycle;
 - ✓ Ionization term in 2nd cycle for j+1th time iteration with results of jth iteration
- Lackner et al.^[7] prior to Behringer et al. proposed similar algorithm for diffusion only type model of impurity ions
- Lackner et al. model: impurity ion number densities (n,) expressed with time centred Crank – Nicholson method as well
- Although ionization & recombination terms alternatively were expressed as 'explicit' or 'implicit' (i.e. jth or j+1th time iteration)
 - **Ionization** terms **implicit** and **recombination** terms **explicit j**th **iteration** \checkmark
 - **Ionization** terms **explicit** and **recombination** terms **implicit j+1**th **iteration** \checkmark

[7] Lackner, K., Behringer, K., Engelhardt, W., Wunderlich, R., 'An algorithm for the description of impurity diffusion under finite reaction rates', Zeitschrift für Naturforschung, 37a(5), pp. 931–938, 1982

A Semi-implicit numerical method for solving the RITE (5/10)

Disadvantages of the earlier numerical schemes for solving the RITE

- Mackenzie and Madzvamuse^[8] on Stability, Convergence of time related numerical methods for the conservative and non-conservative formulations of diffusion-reaction system
- Crank–Nicholson method reported conditionally stable for non–conservative formulation of the governing PDE^[8]
- Time-centred Crank-Nicholson method when applied to RITE with coarse Δt : **Oscillations in solutions transpire; further augment through time iterations**
- Oscillations in implicit scheme mitigated, accuracy comparable to explicit method with chosen Δt lower than required for explicit counterpart
- Crank–Nicholson method in STRAHL unconditionally stable for all Δt ; yet separate time treatment in S_{n_7} necessitate a stability condition (??)

[8] Mackenzie, J. A., Madzvamuse, A., 'Analysis of stability and convergence of finite-difference methods for a reactiondiffusion problem on a one-dimensional growing domain', IMA J. Numer. Anal., 31, 212–232, 2011

A Semi-implicit numerical method for solving the RITE (6/10)

The applied novel numerical scheme for solving the RITE

Ordinary differential equation:

$$f' = \lambda g (f, t)$$
 $f_{j+1} = f_{j+1}$

$$[1 - \lambda K \Delta t] f_{j+1} = [1 - \lambda K \Delta t]$$

 $f_i + \lambda \Delta t g (f, t)$ • The function g (f, t) described as: $g(f, t) = K f_{i+1} + L f_i$ The semi-implicit formulation^[9] of the ODE $-\lambda L \Delta t$] f_i **Implicit terms (j+1th)** (j+1th time iteration) **Explicit terms (jth)** (jth time iteration) Diffusion **Convective velocity Ionization (Z-1) Ionization (Z) Time based semi-implicit Recombination (Z+1) Recombination (Z)** formulation of the RITE **Charge Exchange (Z)** Charge Exchange (Z+1)

[9] Lerbinger, K., Luciani, J. F., 'A New Semi-implicit method for MHD Computations', Journal of Computational Physics, 97, pp. 444–459, 1991

A Semi-implicit numerical method for solving the RITE (7/10)

Terms assigned as 'IMPLICIT' and 'EXPLICIT' upon central-difference (CD) discretization of the radial derivatives (kth node)



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A Semi-implicit numerical method for solving the RITE (8/10)

Forward Differencing (FD) of the time derivative on the LHS of the transport equation:



FINAL FORM of the linearized semi-implicit RITE (The ranges are: $0 < r < r_{0}$; $0 < t \le t_{s}$; Z = 1, 2, 3...N)

$$\left\{ \Delta t \left\{ \frac{D_{k}}{(\Delta r)^{2}} + \frac{D_{k+1}}{4(\Delta r)^{2}} - \frac{D_{k-1}}{4(\Delta r)^{2}} + \frac{D_{k}}{2r_{k}\Delta r} \right\} n_{z} |_{k+1}^{j+1} - \left\{ 1 + \frac{2D_{k}\Delta t}{(\Delta r)^{2}} + n_{e,k}S_{z,k}\Delta t + n_{e,k}\alpha_{z,k}\Delta t \right\} n_{z} |_{k}^{j+1} + \Delta t \left\{ \frac{D_{k}}{(\Delta r)^{2}} - \frac{D_{k+1}}{4(\Delta r)^{2}} + \frac{D_{k-1}}{4(\Delta r)^{2}} - \frac{D_{k}}{2r_{k}\Delta r} \right\} n_{z} |_{k-1}^{j+1} \right\} = \left\{ \begin{array}{c} \frac{\frac{v_{k}}{2\Delta r}\Delta t n_{z} |_{k+1}^{j} - v_{k+1}|}{1 + \Delta t \left[\frac{v_{k-1}}{2\Delta r} - \frac{v_{k}}{r_{k}} - \frac{v_{k+1}}{2\Delta r} \right] \right\} n_{z} |_{k}^{j} - v_{k}^{j} -$$

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$$|| - n_z |_k^j$$

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(BACK)

A Semi-implicit numerical method for solving the RITE (9/10)

Numerical scheme for the applied boundary conditions

• At r = r_o (plasma edge), an explicit three point upwind scheme is used for the decay equation given as:



• At r = 0 (plasma centre) the boundary condition with Forward Differencing (FD): dn_z $\frac{dr^2}{dr}\Big|_{r=0} = 0, \text{ for all } 0 \le t \le t_s \blacksquare$

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$$\frac{1}{\left(3+\frac{2\Delta r}{l_{d}}\right)} = -\frac{n_{z}|_{r=r_{o}}}{l_{d}}$$

$$\frac{1}{\left(3+\frac{2\Delta r}{l_{d}}\right)} n_{z}|_{r=r_{o}-2\Delta r} = 0$$

$$\left(\left.\left(n_{z}\right|_{r=0}-n_{z}\right|_{r=\Delta r}\right)=0$$

A Semi-implicit numerical method for solving the RITE (10/10) **The development in the State–Of–The–Art**

Linearized Semi–Implicit Radial Impurity Transport Equation (SI–RITE):

- ✓ Single time treatment;
- \checkmark Terms remain either implicit or explicit based on phenomena (diffusion, convection, ionization, recombination) and charge state Z

• Advantage:

- \checkmark Prevents interchange of explicit/implicit treatment of terms in S_n, in between consecutive time cycles
- \checkmark No. of cycles reduced to one for any jth time iteration; contrary to multiple cycles for single time iteration in earlier/existing methods
- Single cycle Single time iteration reduces computation time and effort when equation needs solving for smaller Δt
- Following stability condition would ensure numerically stable and convergent solutions of the modelled RITE
- Stability condition derived using a von Neumann stability analysis
- The condition derived must be ascertained for every change in input parameters

The von Neumann stability analysis **Stability analysis of the linearized Semi-implicit** formulation of the RITE (1/6)

Bhattacharya, A., Munshi, P., Ghosh, J., Chowdhuri, M. B., 'A study of the von Neumann stability analysis of a semi-implicit numerical method applied over the radial impurity transport equation in tokamak plasma', Journal of Fusion Energy, 37(5), 211–237, 2018

- A von Neumann stability analysis is a necessary and sufficient test of stability as per the 'Lax Equivalence theorem'
- A generic representation of the Lax equivalence theorem^[10]

"if the original continuous problem is uniquely solvable and well-posed, and if its finite-difference approximation is consistent, then stability of the approximation is necessary and sufficient for its convergence"

- Stability condition determined with the von Neumann stability analysis for the linearized, semi-implicit formulation of the RITE
- Stability analysis performed over $0 < r < r_0$ i.e. plasma boundaries excluded

[10] Ryaben'kii, V. S., Tsynkov, S. V., A Theoretical Introduction to Numerical Analysis, CRC Press, 2006

The von Neumann stability analysis Stability analysis of the linearized Semi-implicit formulation of the RITE (SI–RITE) (2/6)

(BRIEF RECOLLECTION)

The coefficients on the left (**A**, **B**, **C**) and right hand side (**D**, **E**, **F**, **G**, **H**) of the linearized transport equation are identified as:

$$\begin{split} A &= \Delta t \Big\{ \frac{D_k}{(\Delta r)^2} + \frac{D_{k+1}}{4(\Delta r)^2} - \frac{D_{k-1}}{4(\Delta r)^2} + \frac{D_k}{2r_k A} \\ B &= - \Big\{ 1 + \frac{2D_k \Delta t}{(\Delta r)^2} + n_{e,k} S_{z,k} \Delta t + n_{e,k} \alpha_{z,k} \\ C &= \Delta t \Big\{ \frac{D_k}{(\Delta r)^2} - \frac{D_{k+1}}{4(\Delta r)^2} + \frac{D_{k-1}}{4(\Delta r)^2} - \frac{D_k}{2r_k A} \Big\} \end{split}$$



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The von Neumann stability analysis **Stability analysis of the linearized Semi-implicit** formulation of the RITE (SI–RITE) (3/6)

 The linearized, semi-implicit formulation of the radial impurity transport equation for tokamak plasma can be expressed as:

$$\begin{aligned} A n_{z} |_{k+1}^{j+1} + B n_{z} |_{k}^{j+1} + C n_{z} |_{k-1}^{j+1} = \\ D n_{z} |_{k+1}^{j} + E n_{z} |_{k}^{j} + F n_{z} |_{k-1}^{j} + G n_{z-1} |_{k}^{j} + H n_{z+1} |_{k}^{j} \end{aligned}$$

(j – time iteration, k – radial node, Z = 1, 2, 3,....N)

- **Assumptions**^[11]: Numerical error δn associated with n_{2} (ionization state Z = 1, 2, 3,...N) propagating through time iterations are:
 - Exponential in time, periodic in space
 - \checkmark δn for all impurity ionization state is same i.e. $\delta n_z|_k^J = \delta n_{z-1}|_k^J = \delta n_{z+1}|_k^J$
- Wave number $k_m = \pi m/r_0$, where wave mode number $m = 1, 2...r_0/\Delta r$

[11] Moin, P., Fundamentals of Engineering Numerical Analysis, 2nd edition, New York, USA: Cambridge University Press, 2010

The von Neumann stability analysis **Stability analysis of the linearized Semi-implicit** formulation of the RITE (SI–RITE) (4/6)

• Amplification factor **σ** for the numerical error propagating:

$$\sigma = \frac{\delta n_z |_k^{j+1}}{\delta n_z |_k^j} = \frac{e^{a(t+\Delta t)}e^{ik_m r}}{e^{at}e^{ik_m r}} = e^{at}e^{ik_m r}$$

• Error remains bounded iff $|\sigma| \le 1$; **Condition for stability** of SI–RITE ensuring the error propagating remains bounded:

$$|\sigma| = \left| \frac{\mathbf{E} + \mathbf{G} + \mathbf{H} + (\mathbf{D} + \mathbf{F})\cos(\mathbf{k}_{m}\Delta \mathbf{r}) + i(\mathbf{D} - \mathbf{F})\sin(\mathbf{k}_{m}\Delta \mathbf{r})}{\mathbf{B} + (\mathbf{A} + \mathbf{C})\cos(\mathbf{k}_{m}\Delta \mathbf{r}) + i(\mathbf{A} - \mathbf{C})\sin(\mathbf{k}_{m}\Delta \mathbf{r})} \right| \le 1$$

• Following Euler's identity and substituting expressions of coefficients A to H:

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		ſ	j-1, j, j+1 as time iterations;
e ^{a∆t}	with	4	k-1, k, k+1 as radial nodes;
			Z = 1,2, 3, N

The von Neumann stability analysis **Stability analysis of the linearized Semi-implicit** formulation of the RITE (5/6)

• The local maximum value of the time step Δt_{loc} over each kth node, along plasma radius, decided by $|\sigma| = 1$

0/

Local maximum time step Δt_{loc} at each radial (kth) node expressed as:

$$\Delta t_{loc} = 2 \frac{\begin{bmatrix} \frac{2D_{k}}{(\Delta r)^{2}}(1 - \cos(k_{m}\Delta r)) + n_{e,k}S_{z,k} + n_{e,k}\alpha_{z,k} - n_{e,k}S_{z-1,k} - n_{e,k}S_{z-1,k} - n_{e,k}\alpha_{z+1,k} + \frac{v_{k}}{r_{k}} + \frac{v_{k+1}}{2\Delta r} - \frac{v_{k-1}}{2\Delta r} \end{bmatrix}}{\begin{bmatrix} \left(\frac{v_{k-1}}{2\Delta r} - \frac{v_{k}}{r_{k}} - \frac{v_{k+1}}{2\Delta r} + n_{e,k}S_{z-1,k} + n_{e,k}\alpha_{z+1,k}\right)^{2} - \left(\frac{2D_{k}}{(\Delta r)^{2}}(1 - \cos(k_{m}\Delta r)) + n_{e,k}S_{z,k} + n_{e,k}\alpha_{z,k}\right)^{2} + \left[\left(\left(\frac{v_{k}}{\Delta r}\right)^{2} - \left[\frac{D_{k+1}}{2(\Delta r)^{2}} - \frac{D_{k-1}}{2(\Delta r)^{2}} + \frac{D_{k}}{r_{k}\Delta r}\right]^{2}\right) \sin^{2}(k_{m}\Delta r) \right] \end{bmatrix}$$

where, $0 < r_{k} < r_{o}$, $m = 1, 2, 3...r_{o}/\Delta r$ and $Z = 1, 2, 3...N$ with $k_{m} = 0$

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(π m)/r_o **`**m

The von Neumann stability analysis **Stability analysis of the linearized Semi-implicit** formulation of the RITE (6/6)

The stability condition (upper limit to choice time step) for the semi-implicit formulation of radial impurity transport equation (SI-RITE) is given as:



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(ANALOGY)

$$[2]_{Z=1,2,3..N} \Big|_{r \in (0,r_0)} \Big|_{m=1,2,...r_0/\Delta r}$$

 $\forall \Delta t_{loc} > 0$ (i.e. only positive values considered)

minimum of all positive Δt_{loc} values between Z = 1 to Z = N for all radius ($0 < r < r_{o}$) and wave mode number ($1 \le m \le r_{o}/\Delta r$)

minimum of all positive 1st minimum Δt_{loc} values between r > 0 to r < r_o

minimum of all positive 2^{nd} minimum Δt_{loc} values between m = 1 to m = $r_o /\Delta r$

The von Neumann stability analysis

Comparison with the von Neumann stability condition derived for an explicit Forward Euler formulation of the RITE (1/3)

Bhattacharya, A., Munshi, P., Ghosh, J., Chowdhuri, M. B., 'A study of the von Neumann stability analysis of a semi-implicit numerical method applied over the radial impurity transport equation in tokamak plasma', Journal of Fusion Energy, 37(5), 211–237, 2018

 Initial FTCS discretization of the derivatives in RITE; RITE constituent terms next expressed in jth time iteration

$$n_z|_{k,j+1} = n_z|_{k,j} + \Delta t$$

Final explicit formulation of the non–conservative RITE

$$n_{z}|_{k,j+1} = \begin{pmatrix} \left[\frac{D_{k+1}}{4\Delta r^{2}} + \left(\frac{1}{\Delta r^{2}} + \frac{1}{2r_{k}\Delta r}\right)D_{k} - \frac{D_{k-1}}{4\Delta r^{2}} - \frac{v_{k}}{2\Delta r}\right]n_{z}|_{k+1,j}\Delta t + \\ \left[1 - \Delta t \left\{\frac{2D_{k}}{\Delta r^{2}} + \frac{v_{k+1}}{2\Delta r} + \frac{v_{k}}{r_{k}} - \frac{v_{k-1}}{2\Delta r} + n_{e,k}S_{z,k} + n_{e,k}\alpha_{z,k}\right\}\right]n_{z}|_{k,j} + \\ \left[\frac{-D_{k+1}}{4\Delta r^{2}} + \left(\frac{1}{\Delta r^{2}} - \frac{1}{2r_{k}\Delta r}\right)D_{k} + \frac{D_{k-1}}{4\Delta r^{2}} + \frac{v_{k}}{2\Delta r}\right]n_{z}|_{k-1,j}\Delta t + \\ n_{e,k}S_{z-1,k}n_{z-1}|_{k,j}\Delta t + n_{e,k}\alpha_{z+1,k}n_{z+1}|_{k,j}\Delta t \end{pmatrix}$$

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 $t \{R. H. S._{RITE}\}_i$

The von Neumann stability analysis **Comparison with the von Neumann stability condition derived** for an explicit Forward Euler formulation of the RITE (2/3)

• The local maximum time step $\Delta t_{loc, exp}$ for explicit formulation of radial impurity transport equation, analogous to previous format yields:

$$\Delta t_{loc,exp} = 2 \frac{\left[\frac{2D_{k}}{(\Delta r)^{2}}(1 - \cos(k_{m}\Delta r)) + n_{e,k}S_{z,k} + n_{e,k}\alpha_{z,k} - n_{e,k}S_{z-1,k} - n_{e,k}S_{z-1,k} - n_{e,k}\alpha_{z+1,k} + \frac{v_{k}}{r_{k}} + \frac{v_{k+1}}{2\Delta r} - \frac{v_{k-1}}{2\Delta r}\right]}{\left[\frac{\left(\frac{2D_{k}}{\Delta r^{2}}(1 - \cos(k_{m}\Delta r)) + \frac{v_{k+1}}{2\Delta r} + \frac{v_{k}}{r_{k}} - \frac{v_{k-1}}{2\Delta r} + n_{e,k}S_{z,k} + n_{e,k}\alpha_{z,k} - n_{e,k}S_{z-1,k} - n_{e,k}\alpha_{z+1,k}\right)^{2} + \left[\frac{\left(\frac{D_{k+1}}{2\Delta r^{2}} + \frac{D_{k}}{r_{k}\Delta r} - \frac{D_{k-1}}{2\Delta r^{2}} - \frac{v_{k}}{\Delta r}\right)^{2}\sin^{2}(k_{m}\Delta r)\right]}{\left[\left(\frac{D_{k+1}}{2\Delta r^{2}} + \frac{D_{k}}{r_{k}\Delta r} - \frac{D_{k-1}}{2\Delta r^{2}} - \frac{v_{k}}{\Delta r}\right)^{2}\sin^{2}(k_{m}\Delta r)\right]}$$

The upper limit of time step Δt_{exp} for the explicit formulation is given as:

[on

$$\Delta t \leq \Delta t_{exp}$$
 where,
$$\Delta t_{exp} = \min \left[\min \left[\min \left(\Delta t_{loc,exp} \right) \right] \right]$$

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Т

The von Neumann stability analysis **Comparison with the von Neumann stability condition derived** for an explicit Forward Euler formulation of the RITE (3/3)

• Δt_{diff} : Difference between critical times steps Δt_{crit} and Δt_{exp}	Difference Δt _{diff} between the critical time steps for the semi–implicit and the explicit Forward–Euler formulation of the Radial Impurity Transport Equation (RITE)								
$\Delta t_{abc} = \Delta t_{abc} - \Delta t_{abc}$	(A. Bhattacharya et al., Journal of Fusion Energy, 37(5), 211–237, 2018)								
	D	1.5 m²/s	3.0 m²/s	5.0 m²/s	10.0 m²/s	20.0 m²/s	30.0 m²/s	Var. D	
 No. of negative Δt_{diff} values decreases 	Δr (m)	Δt _{diff} (s)	Δt _{diff} (s)	∆t _{diff} (s)	Δt _{diff} (s)	Δt _{diff} (s)	Δt _{diff} (s)	∆t _{diff} (s)	
with increase in impurity diffusivity	5.00E-02	NA	NA	NA	8.679E-04	1.350E-04	NA	1.473E-05	
Diffusivity raducad prominance of	4.00E-02	NA	NA	NA	4.199E-04	3.611E-05	NA	2.253E-04	
[•] Diffusivity reduced, profilmence of	2.50E-02	NA	2.385E-04	7.584E-04	1.680E-04	-2.440E-06	1.561E-04	2.487E-04	
explicit side of SI–RITE: restricts choice	2.00E-02	3.765E-04	4.148E-05	4.911E-06	6.451E-06	2.706E-07	-4.179E-07	2.436E-04	
of Δt; method then computationally	1.00E-02	6.696E-05	-1.539E-07	1.161E-06	1.778E-07	5.986E-07	2.346E-06	7.935E-07	
extensive	5.00E-03	6.116E-07	2.374E-07	6.371E-07	6.994E-08	1.235E-07	1.368E-07	-6.325E-08	
	4.00E-03	-2.313E-08	8.211E-08	1.920E-09	-1.830E-08	1.914E-08	1.225E-08	-7.975E-08	
 Method applicable for diffusion as 	2.50E-03	2.470E-08	-1.131E-07	-2.315E-08	-6.205E-08	2.103E-08	1.345E-08	1.650E-07	
dominant phenomenon	2.00E-03	1.701E-08	-1.502E-08	4.215E-09	-1.924E-08	1.214E-08	1.010E-08	-4.571E-10	
	1.00E-03	-1.677E-08	1.617E-08	1.219E-08	2.155E-08	2.612E-09	1.392E-09	7.928E-09	
• Motivation :	5.00E-04	-6.013E-09	2.576E-09	2.614E-09	5.290E-09	6.269E-10	3.219E-10	2.436E-09	
✓ Stable solutions with greater accuracy over	4.00E-04	-3.916E-09	1.538E-09	1.640E-09	3.378E-09	3.991E-10	2.040E-10	1.377E-09	
existing methods at coarser At	2.50E-04	-1.561E-09	5.540E-10	6.261E-10	1.316E-09	1.549E-10	7.884E-11	4.612E-10	
	2.00E-04	-2.867E-10	3.476E-10	3.984E-10	8.416E-10	9.892E-11	5.032E-11	2.837E-10	
 Wethod applied must be computationally 	1.00E-04	-2.546E-10	8.445E-11	9.853E-11	2.100E-10	2.459E-11	1.253E-11	6.695E-11	
less extensive than explicit counterparts									

Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (1/8)

experimental and STRAHL simulated O⁴⁺ emissivity profiles

Bhattacharya, A., Ghosh, J., Chowdhuri, M. B., Munshi, P., 'Numerical estimation of the oxygen impurity transport in the Aditya tokamak', *Physics of Plasmas*, 27(2), 023303, 2020

- Plasma shot analysed: **#19085**;
- Chord—integrated brightness measured: 650.024 nm characteristic (2p3p³D₃-**2p3d³F₄) transition** of Be –like O⁴⁺ ions ^[12]
- Light collected simultaneously along 8 Lines–Of–Sight (LOS):
 - ✓ Four inboard (high field); Four outboard (low field)
 - ✓ Multi–track spectrometer system

Lens **High-Field** (Inboard side Toroidal

Zones

Chowdhuri M. B., Ghosh, J., Banerjee, S., Dey, R., Manchanda, R., Kumar, V., et al., 'Investigation of oxygen impurity transport [12] using the O⁴⁺ visible spectral line in the Aditya tokamak', *Nuclear Fusion*, 53, 023006, 2013

Benchmarking of the Semi-implicit RITE results against the

Experimental set-up



Analysed shot #19085 in the

Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (2/8)

Benchmarking of the Semi-implicit RITE results against the experimental and STRAHL simulated O⁴⁺ emissivity profiles

- Chord–integrated brightness (B) acquired at 45 ms in discharge, exposure time 10 ms
- Measured data fit to Gaussian curve; Chord– integrated brightness: area under the curve fit
- Radial emissivity profiles (E) from chord– integrated brightness; Abel–like matrix inversion
- Max. ±15% uncertainty in emissivity (E) data upon matrix inversion; radial & angular dependence (poloidal asymmetry) considered
- SI–RITE results with $\Delta r = 0.002 \text{ m}$, v₋= 0.001 m/s; decay length (boundary condition) $I_d = 0.01 \text{ m}$
- Outcome of modelling based on simulated 'best– fit' 650.024 nm emissivity profiles:

✓ Impurity diffusion coefficient (D)

 \checkmark Impurity concentration with respect to plasma density



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Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (3/8)

Benchmarking of the Semi-implicit RITE results against the experimental and STRAHL simulated O⁴⁺ emissivity profiles

Time steps Δt for SI–RITE along inboard and c

Upper limit to time step Δt_{crit} (s)

Time step chosen Δt (s)

- <u>Diffusivity (inboard/outboard) profiles</u>: Constraining 'simulated' radial 650.024 nm O⁴⁺ emissivity profile to **'experimental'** emissivity data
- Oxygen ion diffusivity profiles (inboard/outboard) concluded based on 'best-fit' simulated radial (650.024 nm) emissivity profiles
- Radial emissivity profiles of characteristic impurity ion transitions from n, profiles of both STRAHL and Semi–Implicit RITE

$$E_{z}(r) = \frac{\begin{pmatrix} n_{e}(r) \ n_{z,g}(r,t = t_{s}) \ PEC_{z}^{exc}(r) + n_{e}(r) \ n_{z+1,g}(r,t = t_{s}) \ PEC_{z+1}^{rec}(r) \\ n_{i0}(r) \ n_{z+1,g}(r,t = t_{s}) \ PEC_{z+1}^{cx}(r) \\ 4\pi$$

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outboard regions of the Aditya plasma				
Inboard	Outboard			
3.837E-08	7.837E-09			
3.750E-08	7.750E-09			



- n_{z,g} and n_{z+1,g} : 'Ground state' impurity ion (Z and Z+1) number densities
- 'Excitation' PECs only considered (Aditya T_e profile, no neutral beam heating)
- **PECs from ADAS database; extrapolated** based on Aditya n_e and T_e profiles

Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (4/8)

Comparison between the profiles from two separate impurity transport solvers STRAHL & SI-RITE

(A. Bhattacharya et al., *Physics of Plasmas*, 27(2), 023303, 2020)



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Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (5/8)

Analysis of the anomalous transport at the Aditya plasma edge

- Large impurity diffusivity values at plasma edges; cannot be explained with standard neoclassical theory (D ~ 1.5 m²/s); fluctuation–induced edge impurity transport confirmed!
- Edge fluctuations attributed to instabilities; each with characteristic region of dominance based on plasma temperature ^[13]
 - Resistive ballooning mode: Lowest temperature (edge) region; destabilizing field curvature due to larger pressure gradient
 - \checkmark **Ion temperature gradient (ITG) or** η_i **modes:** High temperature region with steep gradient

<u>Condition for dominance of η_i (ITG) turbulence modes over Resistive Ballooning (RB) modes ^[13]</u>:

$$\frac{\rho_s^2}{L_\perp^2} = \epsilon_n \alpha_d^2 (1+\tau)^2 > 1 > \frac{1}{q} \left(\frac{L_p}{R}\right)^{\frac{1}{4}} \sim k_\perp \rho_s$$

where,
$$c_s^2 = \frac{(T_{io} + T_{eo})}{m_i}$$
; $\rho_s = \frac{c_s}{\Omega_{ci}}$; $t_o = \left(\frac{RL_n}{2}\right)$
$$L_{\perp} = 2\pi q_a \left(\frac{\nu_{ez} R \rho_s}{2 \Omega_{ce}}\right)^{\frac{1}{2}} \left(\frac{2R}{L_n}\right)^{\frac{1}{4}}$$
; $\Omega_{ce} = \frac{eB}{m_e}$

[13] Zeigler, A., Biskamp, D., Drake, J. F., Rogers, B. N., 'Transition from resistive ballooning to η_i driven turbulences in tokamaks', *Physics of Plasmas*, 5(7), 2654–2663, 1998

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1 $\frac{1}{c}; \alpha_d = \frac{\rho_s c_s t_o}{(1+\tau) I_{-} I_{-}}; \epsilon_n$ 2 eo ; $\Omega_{ci} = \frac{(Ze) B}{m_i}$; $\nu_{ez} = \frac{4 \sqrt{2\pi} e^4 Z^2 (\ln \Lambda) n_Z}{3 (4\pi\epsilon_0)^2 m_0^{1/2} T_0^{3/2}}$;

Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (6/8)

Comparison between the simulated diffusivity values and the values from an analytical model at the edge regions of Aditya plasma

- Growth rate (RB; ITG mode) $\gamma \sim c_s / (L_p R)^{1/2}$ peaks to same intensity; Difference in scale lengths at which y peaks
- Drift resistive ballooning mode diffusivity ^[14]:

$$\mathbf{D}_{RB} = \mathbf{C}_{RB} \left(2\pi q_a\right)^2 \mathbf{v}_{ez} \rho_e^2 \left(\frac{\mathbf{R}}{\mathbf{L}_p}\right) \sim$$

• Diffusivity perpendicular to the magnetic surface due to ITG modes:

$$D_{ITG} \sim \frac{c_s \rho_s^2}{(L_p R)^{1/2}} \left(\frac{q^4 R}{L_p}\right)^{1/4}$$
 [13] A. 2

Parameters for estimating fluctuation induced transport alo (A. Bhattacharya et al., *Physics of*

r _o (m)	R _o (m)	q _a	T _{e.0} (eV)	T _{i.0} (eV)	m _i (kg)	e (C)	L _n (m)	L _p (m)
0.25	0.75	4.0	350	350	2.672E-26	1.602E-19	0.009	0.009
ρ _{e, ro} (m)	C _{RB}	v _{ez, ro} (s⁻¹) INBOARD	Ω _{ce, ro} (s ⁻¹)	Ω _{ci, ro} (s ⁻¹)	v _{ez, ro} (s⁻¹) OUTBOARD	c _s (m/s)	ρ _s (m)	τ
1.484E-05	14	3.717E+04	1.413E+11	1.928E+07	4.214E+04	6.479E+04	3.361E-03	1
[14] Redd, A. J., Kritz, A. H., Bateman, G., Kinsey, J. E., 'Sensitivity of predictive tokamak plasma transport simulations', <i>Physics of Plasmas</i> , 4(6), 2207–2214, 1997								

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\frac{L_{\perp}^2}{t} where, 10 < C<sub>RB</sub> < 30<sup>[14]</sup>
```

Zeigler et al., *Physics of Plasmas*, 5(7), 2654–2663, 1998

ng inboard and outboard edges of the Aditya tokamak	
Plasmas, 27(2), 023303, 2020)	

Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (7/8)

Comparison between the simulated diffusivity values and the values from an analytical model at the edge regions of Aditya plasma

(A. Bhattacharya et al., *Physics of Plasmas*, 27(2), 023303, 2020)

Parameters calculated at the Aditya plasma edge ($r = r_0$) for analysing edge fluctuation induced transport

	€ _n	t _o (s)	L⊥ (m)	$\boldsymbol{\alpha}_{d}$	$S_{LHS} = \epsilon_n \alpha_d^2 (1+\tau)^2$	S _{RHS} =	(1/q) (L _p /R) ^{1/4}
Inboard	0.036	7.321E-07	1.213E-03	7.302	7.678	>>	0.092
Outboard	0.018	1.035E-06	2.172E-03	5.767	2.394	>>	0.077
R = R –	r _o for the	inboard section	on and R = R +	r _o for the	outboard section at th	e plasm	a edge
(Cor	ndition f	or dominan	ce of ITG m	odes ove	e <mark>r RB modes: S_{LHS} ></mark>	>> 1 >>	S _{RHS})
Diffusion coefficients of the oxygen ions at inboard and outboard plasma edges (r = r _o) of Aditya tokamak							
	21 ,2/+	П	$(m^2/s) \sim$		D (n	n²/c)~	

	2L⊥ ² / t _o (m²/s)	$D_{RB} (m^2/s) \sim C_{RB} (2\pi q_a)^2 v_{ez} \rho_e^2 (R/L_p)$	D _{ITG} (m²/s)	$D_{ITG, FINAL} (m^2/s)^{2}$ $(L_{\perp}^{2}/\rho_{s}^{2}) D_{ITG}$	D (m²/s)
Inboard	4.020	4.020 <<	119.164	15.520	19.540
Outboard	9.115	9.115 🕇 <<	100.204	41.852	50.967
R = R -	r _o for the in	board section and R = R + r _o f	for the outboard	l section at the plasma e	edge
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Estimation and analysis of the impurity diffusivity values at the edge regions of the Aditya plasma (8/8)

Comparison between the simulated diffusivity values and the values from an analytical model at the edge regions of Aditya plasma

• D_{ITG} absurdly large value for edge diffusivity; expression multiplied by factor $\left(\frac{L_1^2}{Q_2^2}\right)$

$$D_{\text{ITG,FINAL}} = \left(\frac{L_{\perp}^2}{\rho_s^2}\right) \frac{c_s \rho_s^2}{\left(L_p R\right)^{1/2}}$$

Diffusion coefficients of the oxygen ions at the plasma edge $r = r_0$ along inboard and outboard sections of Aditya tokamak

	2L⊥ ² / t _o (m²/s)	$D_{RB} (m^2/s) \sim C_{RB} (2\pi q_a)^2 v_{ez} \rho_e^2 (R/L_p)$	
Inboard	4.020	4.020	
Outboard	9.115	9.115	

 $R = R - r_o$ for the inboard section and $R = R + r_o$ for the outboard section at the plasma edge

- Edge diffusivities with STRAHL results: D ~ 19 m²/s at ρ = -1.00 (inboard); D ~ 44 m²/s at $\rho = +1.00$ (outboard)
- Edge diffusivities with SI–RITE results: D ~ 19 m²/s at ρ = -1.000 (inboard); D ~ 51 m²/s at $\rho = +1.000$ (outboard)

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 $\frac{1}{1/2} \left(\frac{q^4 R}{L_n}\right)^{1/4}$ wavelength of the ITG modes >> Ion Larmor radius !



Conclusions

- Novel application of semi-implicit numerical method for solving the Radial Impurity Transport Equation (RITE) for tokamak plasma
- SI-RITE novel contribution to the <u>state -of-the-art</u>; Single cycle-single time iteration approach in the applied semi-implicit method:
 - ✓ Reduces computation time for smaller time steps
- The von Neumann stability analysis presented unlike earlier methods
 - Performed over realistic cylindrical coordinates (and not slab geometry) \checkmark
 - All relevant terms (transport coefficients, ionization and recombination) of the radial impurity \checkmark transport equation taken into consideration
 - Allows application of the method with greater accuracy at coarser time steps \checkmark
- Simulated 650.024 nm O⁴⁺ emissivity profiles matched with experimental data from Aditya tokamak

✓ ITG driven transport dominate over RB modes RB in both regions of Aditya plasma

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