Scientific Proposal for a Theory Simulation Verification and Validation (TSVV) Project

Topic	**TSVV-K: Neutral Particle Models**
Principal Investigator	***Dmitriy V. Borodin***
Lead Beneficiary	***FZJ***

Abstract

Neutral gas physics and its interactions with the plasma are key aspects of edge plasma and divertor physics in present fusion devices, and to much greater extent for next-step fusion devices, such as ITER and DEMO. This proposal foresees the development, verification and validation of a hierarchy of Neutral Gas Models, the full physics version being based on the existing neutral gas module (NGM) – the 3D Monte-Carlo (MC) Boltzmann-equation EIRENE code in the continuity of TSVV5; EIRENE already includes advanced fluid neutrals (AFN) and various fluid-kinetic hybridisation (FKH) reduced modes, approaching the accuracy of the full-kinetic runs, while providing a treatment of particular (e.g. high collisional) domains or regimes. The goal is for the NGMs to be employable in any 2D, 3D and ultimately 5D simulations of reactor-relevant regimes with (semi)detached divertor on ITER and DEMO scale. The interfaces to other codes are liaised with TSVV-B&C, on the basis of the STYX2.0 interface (co-developed with TSVV-3). In terms of physics, the project will enable full physics time-dependent simulations both for neutral particle transport and recycling processes. At lower fidelity levels, advanced neutral fluid models will be extended to molecules, whose transport significantly differs from that of atoms. Hybrid kinetic fluid models of the kinetic diffusion Monte-Carlo (KDMC) type will also be further developed as an intermediate level in the hierarchy.

The physics improvements will include refined and extended collisional-radiative models (CRMs) for atoms and molecules (A&M), including resolving the rotational and vibrational states, and treatment of isotope effects for H2, D2, T2, DT and molecular ions. The current CRM in EIRENE will be extended to the hydrogenic isotopes, and their atomic and molecular (A&M) rates will be revised and opacity effects validated against JET-ILW data. The development of the new flexible ModCR collisional-radiative CRM module started in TSVV-5 (mostly just a concept) will be continued to allow for longer term development and modernization of EIRENE e.g. its modularisation. However, ModCR will also allow removal of redundant branching inside the numeric core by A&M process type in the main loop. It will provide flexible transition to algebraic or ODE-based tracing of internal state balance as an alternative to the pure MC approach (sufficient MC particle statistics causes critical memory and performance issues by significant number of the resolved and followed states).

Motivation and context (up to 1 page)

The proposal is summarized as follows:

i) During the last few years, progress has been made in high fidelity edge modelling for plasma codes, with reduced neutral models from TSSV-5 implemented/being implemented [2].

ii) Similarly, progress has been made in developing collisional-radiative models (CRMs) and updating the underlying A&M data. These rates have not yet been transferred to EIRENE or other neutral fluid models. The new ModCR module was concepted, which can critically improve the most performance-demanding A&M side of EIRENE. Moreover, standalone version of ModCR can be seen as a reduced model (pure A&M part neglecting transport) similar to many established outside tools like Yacora [9].

iii) The relevance of full-neutral physics for quantitative comparison between experiments and 2D transport codes has been clearly demonstrated. The latter full physics option is not yet available to 3D fluid turbulence codes, mostly because of memory issues related to the way the coupling is currently done in the model Soledge3X-EIRENE code using the STYX1.0 interface [8].

Next step devices, like ITER and DEMO pose significant challenges, well beyond the increased grid size due to larger machine size. The spatial scales relevant for neutrals are the same as in current devices, but the devices are significantly larger in size. Since the time scale to establish global particle balance for larger devices is much longer than in present devices, it causes major stiffness in the simulations. This issue is exacerbated for the Monte-Carlo approach because of increased collisionality and the size of highly collisional regions.

The ultimate motivation of the NGM development is TSVV-K is to enable full neutral physics simulations for TSVV B-C codes of next-step fusion devices for strongly detached divertor regimes. One key physics gap to close is isotope mixes for which AM physics is incomplete. Systematic measurements in JET-ILW H, D, T and D-T plasmas provide the foundation for validation efforts. The improvements foreseen for AM physics will benefit the 2D transport community also.

HPC machines have evolved towards GPU and so have most of the plasma codes. Neutral fluid models developed in TSVV-5 and implemented in TSVV-B codes will benefit from current GPUisation efforts. Moving the full physics EIRENE code to GPU is not foreseen within 2026-2027 since this is not mandatory to achieve physics goals, and because this requires major algorithmic changes in spite of the embarrassingly parallel nature of the MC (e.g. going towards event-based MC), to ensure performance gain as shown by similar work in other fields (e.g. neutronics). However, it is worth doing in case further ACH support is provided.

Scientific objectives and impact (up to 2 pages)

The first main objective of the project is to enable the inclusion of neutral gas physics in codes developed in TSVV-B and C, from full physics kinetic description to reduced models based on fluid closures. This task is a mandatory step toward predictive simulations of current and future fusion devices, and implies i) further developments of the hierarchy of tools evolved through TSVV-5 with specific efforts to provide a generic interface to fluid, and ultimately gyrokinetic plasma codes but also ii) to close a key gap in the physics available so far, namely the atomic and molecular (A&M) physics for hydrogen isotopes mixes.

The project is thus mostly focused on unlocking full physics neutrals in 3D turbulent fluid codes such as SOLEDGE3X, GRILLIX, FELTOR and preparing such a move for gyrokinetic codes such as GENE-X. Neutrals fluid models based on TSVV-5 results [19] are currently implemented or being implemented in these codes. As shown by the experience with transport codes, quantitative comparison to experiments, especially in reactor relevant regimes (detached plasmas, X-point Radiator (XPR), relies on high fidelity models for neutrals. As a result, a major impact expected from the project is precisely to enable quantitative validation of these codes in reactor relevant regimes and extrapolation towards next-step fusion devices. The continued development of reduced fluid models will enable scoping studies (parametric scans), e.g. investigations for divertor designs, while further development of hybrid fluid-kinetic models will enable computationally feasible, full physics simulations at the reactor scale.

1) Multi-fidelity hierarchy of models

To further enhance the physics models, the focus of the NGM development under TSVV-K is to enable the coupling of the NGM to TSVV-B codes with STYX2.0 as described in the technical aspects of the project implementation, and to introduce time-dependency on neutral transport and recycling. Currently, both fluid and kinetic models assume that the recycling flux follows the incident plasma flux adiabatically. This model is correct for backscattering which occurs on the picosecond scale, but not necessarily the case for the molecular recycling flux, since if there is no time delay in the recycling process molecules will be quickly re-ionized in the filament which produced them, while otherwise they may live and travel much farther. Correcting this requires detailed simulations of the trapping and diffusion mechanisms within the material wall and the derivation of a reduced model applicable both to both fluid, hybrid and kinetic levels in the neutral model hierarchy.

The numerical cost of the full physics EIRENE implementation is addressed by various methods including "brute force" parallelization, which is continuously optimized.

However, the essential progress including on the DEMO scale [4] for most demanding from kinetic side high-collision regions (HCR) is based on the use of fluid approach for neutrals e.g. "Advanced fluid neutral" (AFN) approach or more flexible (but more complex) intermediate option – fluid-kinetic hybridisation (FKH). The hierarchy of various FKH approaches is defined in [2] defining the proposed strategy for the task in TSVV-K. This project will focus on the development of fluid model for molecules, to be used jointly with the AFN developed for atoms so far, and its integration into the FKH currently available in SOLPS. The other important new development will be on kinetic-diffusion Monte-Carlo hybrid models, an alternative which transitions between fluid and kinetic limits within the Monte-Carlo scheme.

2) **High Fidelity CRM models**

An essential part of the NGM are the collisional-radiative models (CRMs) treating multiple A&M processes and involving both main-plasma species and impurities. These processes include ionization-dissociation-recombination and elastic processes. A major issue for simulations at the ITER or DEMO scales is the CPU cost, which is mostly due to the complexity of particle histories on the kinetic side of the EIRENE-CFD packages, in that the A&M processes are responsible for. Another issue is the growing requirements for the A&M data, in both quantity and detail also data type variety which also affects the performance.

A similar argument applies to collisional-radiative models: to further improve the photon opacity module in EIRENE [14] by adding isotopomer reaction data, the project seeks radically improving the main loop by developing a dedicated universal "ModCR" [15] module with new functionality and even mathematical basis containing a flexible transition to ODE solution for balance equations as alternative to pure MC approach. Since ModCR can either be used in standalone or inline mode in other codes than EIRENE, it also serves as a reduced CRM model.

To improve EIRENE-NGM performance issues we propose to refine its atomic and molecular (A&M) physics part – collisional-radiative models (CRM). The new ModCR module for EIRENE, also available as a standalone CRM recently concepted [15], aims to provide a new level of controllability and intrinsic analysis for the A&M data, thus allowing much larger data volumes and type versatility (e.g. resolution by ro-vibrational states demonstrated to be of importance for detachment studies). ModCR allows non-stationary solutions for non-LTE (local thermodynamic equilibrium – for all states i their populations $dN_i/dt=0$) plasmas with strong parameter gradients and tracking of internal states as a population variable "carried" by MC species (flexible alternative to pure MC approach). ModCR is also meant to provide:

- Dynamic changes in the state populations by solving the time-dependent balance equations (ODEs) instead of typically used LTE assumption.
- Critical increases in performance due to the reduced number of MC species to be tracked, substituted by state population variables with a flexible border between both approaches.

The general improvement of the A&M and CRM part in EIRENE as well on the associated external tools and data bases is part of the proposed work. This sub-task includes validation of reaction datasets (both structure and content) in the EIRENE-related CRMs, in view of the prominent role of A&M processes during detachment and of the necessary massive data extension to resolve rovibrational states, which can have impact on global parameters like total ionisation in the volume. The data amount and complexity require improved tools [16] for visualization, processing, and quality/consistency control, such as the web-based toolkit PLOUTOS. The new ModCR code is aimed to eventually substitute both internal and external solvers as well as a significant part of the data processing (DP).

The development of the photon opacity module and the validation of the impact of photon opacity on the ionisation balance in the divertor is an important sub-task of the proposal. The photon transport model in standalone EIRENE was previously applied to JET-ILW L-mode plasma solutions from SOLPS-ITER and revealed the contribution of Ly-β opacity towards D_α emission relative to other processes [14]. The simulations indicate local regions with high Ly-α and Ly-β opacity in high-recycling and detached conditions. This opacity effect is predicted to reduce the Ly-α and Ly-β signals from the low-field side divertor by at least a factor of 2. The contribution of Ly-β to the population density of D (n = 3) is mostly localized near the emission source. In low-recycling regime, Lyman opacity is negligible. Ly-β is dominant in the high-recycling regime with predicted doubling of Dα peak emission values. In the detached regime, contribution from atomic recombination is dominant, but Ly-β capture remains relevant with predicted doubling of Dα emission in the private flux region and 50% enhancement at the strike point. In conclusion, opacity effects must be considered for the analysis of Ly-α, Ly-β and Dα diagnostics in high-recycling and detached conditions. Initial studies showed that the photon absorption has a ~20% effect on the total ionisation in JET volume [14].

The proposal thus contains a validation (following the earlier practices e.g. [17]) and verification part with experiments at JET-ILW and PSI-2. Predictive power and computational performance implications due to the mentioned above improvements will be demonstrated for ITER (focus on semi-detached divertor scenario) and DEMO (focus on HCR) scales. The validation effort will be equally focussed on A&M physics by testing of implications from improved CRM and photon trapping (spectroscopy for well-characterised plasma conditions) updates.

Project description and implementation (up to N pages)

WP0: Overall project management and code maintenance (lead: D.V. Borodin)

In this WP we coordinate the TSVV-K work including the links to partner TSVVs and anticipated support from ACHs. In particular, support for parallelisation and domain decomposition scheme optimisation incl. utilizing EIRON and IMASification will be asked, which cannot be done by the main team due to budget limitations. This task includes maintaining the code (Git) and other repositories (AMNS data, simulation results - SimDB) including the update of the related CI and documentation.

WP1: Establish a multi-fidelity model hierarchy for the physics of neutrals, ranging from first principles models to reduced representations, and integrate it into fluid and gyrokinetic edge turbulence simulations. Exploit synergies with TSVV-B and TSVV-C.

WP1.1 Advanced fluid models (Lead: W. Dekeyser)

The currently available AFN and SpH (Spatially Hybrid) models are based on atom-only models for hydrogenic species (H/D/T) which assume CX as the dominant collision. These models have shown excellent agreement with atom-only kinetic simulations in highly collisional conditions at the reactor scale. At the same time, the effect of including molecules in these regimes is essential. An analysis of the molecule distributions under these conditions shows that they approach near-Maxwellian shapes instantaneously in HCRs, due to ion-molecule collisions. With this basis, the main focus in the project will be on further extension of the AFN model towards molecules, deriving consistent transport coefficients and boundary conditions. Moreover, at the moment only a basic correction for atom-atom self-collisions is available in the AFN models, but needs rigorous extension. The combination of atoms and molecules in the fluid models will greatly enhance their reliability, and offer an accurate, noise-free model for simulations at ITER / DEMO scale and implementation in TSVV-B/C codes. While a full fluid model for molecules sacrifices some accuracy in terms of physics, it is expected to greatly reduce computational cost. Moreover, it is expected to alleviate numerical issues related to particle balance in mixed-species processes (e.g. isotope effects in CX collisions and molecular composition), which currently present a bottleneck for, e.g., D-T simulations. Integration of these extended fluid models in the SpH approach will ensure a correct treatment of kinetic effects in regions and regimes of low collisionality.

WP1.2: Improved Kinetic Diffusion Monte-Carlo (KDMC) (Lead: G. Samaey)

Though KDMC has shown impressive speedups compared to fully kinetic simulations [23], all existing KDMC implementations [6][24][25] share a common issue: the application cases are too simplified to be used in real simulations. Nonetheless, these implementations form a strong foundation, and, in this project, we will build on them so that KDMC is applicable to actual fusion devices. Specifically, we aim to have a KDMC implementation with the following features: complex geometries through the use of a 3D mesh, accurate boundary conditions by connecting with the TRIM database (both for the kinetic and the fluid boundary conditions), full support for heterogeneous plasma backgrounds with physically relevant parameters, and a module that translates EIRENE input to allow users to interface with our code seamlessly. We note that this implementation will still be based on an atom-only model and will therefore miss the important molecular effects mentioned above. Nonetheless, these models will capture important kinetic effects in non-HCR where pure fluid models are less accurate. We will validate the implementation by performing a detailed comparison between our implementation and other codes. Of the different KDMC implementations, our recently developed code NEPTUNE is the closest to achieving these goals and therefore we will choose this code to continue our work. Though this package is relatively new, we are confident that an active effort to find collaborations will be successful once the improvements to the physics are completed.

WP1.3 Interface to CFD codes (Lead: Y. Marandet)

Enabling the use of FKH or fully kinetic models in TSVV-B & C codes requires a flexible interface, which we intend to provide through STYX2.0, the development of which was initiated jointly by TSVV-5 and TSVV-3. Since advanced neutral fluid models will be available in most of the plasma codes of interest, the focus will be on unlocking the use of kinetic models (and thus also to hybrid fluid-kinetic models). The current implementations of STYX1.0 (the original interface between Soledge3X and EIRENE) builds the EIRENE grid (triangles in the poloidal planes) from the plasma solver grid by splitting each quadrangular cell into two triangles. This implementation reduces discretization errors at the interface of the codes but leads to a massive over-resolution for neutrals in most of the computational domain, which has been a major restriction in the last few years. Decoupling the grids will require additional interpolations and using an external gridding tool but is expected to relax to a large extent the memory requirements for EIRENE. Together with the shared memory parallelization layer of EIRENE developed and tested within TSVV-5 and adjustments of the numerical precision of the EIRENE tallies this implementation will allow running Larmor radius resolved turbulence simulations with the full physics EIRENE code on current fusion devices. Exploratory work will continue in parallel on domain decomposition algorithms to be implemented in EIRENE, but this step will become mandatory only later in time when addressing next-step devices at full resolution.

A second important aspect to be addressed is to enable time dependent kinetic simulations with EIRENE, since the stationary approximation used so far is only at best marginally valid on turbulent time scales. This implementation requires further work in the interface and extensive testing to find optimal tuning. It may also have benefits for 2D transport simulations of next-generation devices, such as ITER and DEMO, for which some particles have very long trajectories (e.g. under the dome), the duration of which is much larger than the plasma evolution time. The time scales relevant to the boundary conditions are expected to play an important role and will be explored using the wall model developed by the CEA/AMU team (macroscopic rate equations model, including diffusion and trapping of hydrogen isotopes in the wall). The extension of the model is to better understand the correlations in time between the incident plasma flux and the neutral outgassing.

Efficient coupling of EIRENE to fluid codes requires an assessment of numerical errors and convergence of neutral and coupled plasma-neutral simulations (including turbulence effects) that allows selecting optimal numerical parameters, including mesh size and number of particles [27], optimal particle simulation and estimation techniques [28] and optimal coupling strategies [26]. For this we rely on the expertise of the KU Leuven team. This expertise allows to assess numerical accuracy and accelerating simulations by an appropriate choice of numerical parameters, which is a need in TSVV-C.

WP2: Develop high fidelity collisional-radiative models for H, D, T neutrals further, apply them to mixed fuel plasmas, and assess properties of charge-exchange neutrals.

WP2.1 Development of ModCR and PLOUTOS (lead: D. V. Borodin)

The primary purpose of this sub-task is the general improvement of the A&M and CRM part in EIRENE-NGM as well on the associated external tools and data bases. Validation of reaction datasets (both structure and content) in the EIRENE-related CRMs, in view of the prominent role of A&M processes during detachment and of the necessary massive data extension to resolve ro-vibrational states. The data amount and complexity require improved tools for visualization, processing, and quality/consistency control. The web-based toolkit PLOUTOS is a standard pre-processing tool for EIRENE. It automatically provides the EIRENE input. The PLOUTOS solver is external, thus neglecting the transport effects, but its results can be related (by scaling the particle sources [11]) to the full-scale CFD-EIRENE simulations. The new ModCR code is aimed to eventually substitute both internal and external solvers as well as serving as a data processing tool. The established CRM YACORA [9] is used for verification. A large effort is given to harmonizing the data and assumptions in the various CRMs, as well as demonstration of various particular effects: significance of particular reactions, effect of resolving the vibrational states (available e.g. in [29]), isotopes, etc. The implementation of photon opacity module [14] [9] (from ColRad, see WP2.2) into EIRENE version with ModCR, and the effect of photon transport on opacity and the plasma ionisation balance will be performed and validated against spectroscopic measurements in JET-ILW and PSI-2.

ModCR" [16] is intended to eventually replace both the related routines in the main loop of EIRENE as well as the standalone CRM solvers (e.g. in PLUTOUS), largely improving performance and providing new functionality. It is also aimed to meet the challenge of the exploding amount of molecular data due to the necessity to include the vibrational [16] (and even rotational) states and hydrogen isotopes or atomic states with metastables [13]. ModCR also serves as a module with API in other similar codes like e.g. ERO, assisting interfaces and validation. The primary purpose of ModCR is to provide:

(i) Dynamic changes in the state population instead of typically used local thermodynamic equilibrium (LTE) assumption. The resulting balance equations (ODEs) are solved numerically by CVODE-based routine or MC.

(ii) Critical increases in performance due to the reduced number of MC species to be tracked, substituted by state population variables with a flexible border between both approaches.

(iii) A realistic workload for the EIRON toy-model of EIRENE under development by ACH-VTT, used to evaluate parallelisation, domain decomposition, and fluid-kinetic hybridisation concepts.

WP2.2 Validation with experiment, photon tracing and ColRad development (lead: M. Groth)

To address the impact of hydrogenic isotope-specific charge-exchange rates and photon opacity on the divertor plasma conditions, the EIRENE-internal COLRAD routines will be reactivated and tested against standalone version, such as Sawada/Yacora [9] and ModCR [15]. EIRENE will be refactored to permit flexible inputs of atomic and molecular rates through external data formats, and the existing parameterisation for Te and ne bypassed to directly input Te, Ti, ne and the kinetic energy of the neutrals into the CRM. Pre-conditioning of the CRM will be accomplished via OpenMP parallelisation in collaboration with AMU/CEA. The initial assessment of the impact of the revised physics model will be carried out for D2, using plasma-neutral charge-exchange and molecular-assisted recombination rates from MCCC [29] and [30]. The role of negative hydrogen ion versus deuterium will be elucidated. Provision for extending the implementation toward T2 and the heteronuclear diatomic DT (and HD) will be made.

The impact of photon opacity on the divertor conditions will be assessed in (plasma-neutral) coupled SOLPS-ITER simulations for JET-ILW, Magnum-PSI and PSI-2. Previously, in standalone EIRENE simulations, it was show that the effective ionisation rate in the divertor increased by 25% when opacity is included [14]. The opacity module was implemented in SOLPS-ITER as part of the 2021-2025 TSVV-5 project; the assessment of the impact in coupled SOLPS-ITER simulations is documented and published as part of the PSI 2026 conference.

Similarly, the impact of revised COLRAD routines in (plasma-neutral) coupled SOLPS-ITER simulations will be validated against existing plasma and spectroscopic measurements in JET-ILW plasmas. The validation will draw in measurements from dedicated experiments performed in 2018-19 to infer the molecular and atomic influxes in hydrogen, deuterium, tritium and 40%-60% deuterium-tritium plasmas.

Given these analyses steps, the upgraded physics modules will be applied to SOLPS-ITER simulations to a range of ITER scenarios, and their impact on the power exhaust assessed (in collaboration with ITER IO).

Team members and project management (up to 1 page text, plus CVs)

The project is expected to be contributed by 6 RUs (FZJ is a base). Table below contains the participant list with the PM distribution per year (equally for 2026/27). The principal investigator (PI) as well as RU contact persons (CP) are identified – those build up the management structure.

RU	Name	PM (TSVV-K)	PM (other means)	Total RU	PI/CP
FZJ	Dmitriy Borodin	4	0	10	PI + CP
FZJ	Derek Harting	1			
FZJ	Michael Gordon	5			
DIFFER	Egbert Westerhof	0	0	0	CP
DIFFER	Stijn Kobussen	0			
DIFFER	Pieter Willem Groen	0			
Aalto	Mathias Groth	0	0	9,5	CP
Aalto	Ray Chandra	5			
Aalto	Timo Kiviniemi	4,5			
CAE/AMU	Yannick Marandet	0	0	7	CP
CAE/AMU	Nicolas Rivals	4			
CAE/AMU	Julien Denis	3			
KUL	Wouter Dekeyser	0	0	9,5	CP
KUL	Wim Van Uytven	5			
KUL	Giovanni Samaey	0	0		
KUL	Thijs Steel	4.5			
ENEA	Francesco Cianfrani	0	2 (“AR”)	0	CP
	Total:	36	12*PM = PPY	36	

If further support from the ACH can be secured, further development in IMASification and use of the EIRON for EIRENE as well as in code profiling and improving of the existing hybrid MPI/OpenMP parallelisation scheme and exploration of domain decomposition will be carried out.
The activity was and is expected to be strongly supported by ITER including direct participation of the SOLPS-ITER (same as B2.5-EIRENE) representative in the discussions and events. This is key to avoid divergences in EIRENE version and allow proper integration of developments made within the SOLPS-ITER community.

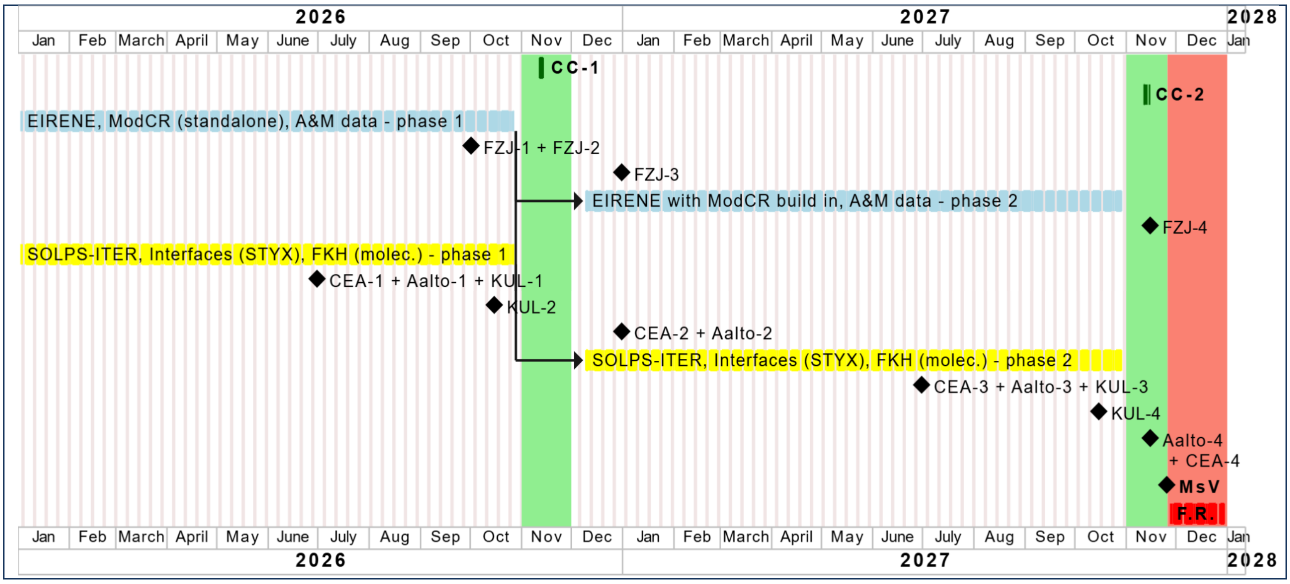
The TSVV-5 experience has proven that a biweekly regular VC with an in-person Code Camp once a year (3 days, typically in November) is a good practice allowing sufficient base communication. Of course this is added up by dedicated VCs, visits between RUs etc.

Work plan (up to 1 page)

Milestones

No	Title	Description	Expected date
1.	FZJ-1	ModCR is fully functional (also validated by applications) as a standalone application, linked with PLOUTOS (data pre-processing web-based tool) and tested with some of the available datasets (most critical ones like H2 or D2)	09/2026
2.	FZJ-2	ModCR is built into EIRENE (as alternative to the available CRM) including the necessary links with COLRAD etc. The performance of the code is tested and the results are verified by applications (sensibility tests). The module is available with API.	09/2027
3.	FZJ-3	The consolidated and well-documented version of the EIRENE ("MsV" – milestone version) containing all of the TSVV-5 and TSVV-K improvements is released after validation, check-up with TSVV-B,C (interfaces) and ITER after last Code Camp in 2027.	11/2027
4.	CEA-1	STYX2.0 interface available to TSVV-B with documentation.	06/2026
5.	CEA-2	STYX2.0 version with capability to run EIRENE on an independent grid (triangles in a poloidal section) available. Demonstration on a high resolution SOLEDGE3X-EIRENE turbulent case.	12/2026
6.	CEA-3	STYX2.0 fully capable of running EIRENE in time dependent mode, including reduced time-dependent recycling model.	06/2027
7	CEA-4	Full neutral physics medium-size tokamak turbulent simulation with SOLEDGE3X-EIRENE in collaboration with TSVV-B.	11/2027
8.	Aalto-1	Validation of photon opacity model in SOLPS-ITER against UV and visible-wavelength range spectroscopic measurements in JET-ILW plasmas.	07/2026
9.	Aalto-2	Verification (against Sawada/Yacora and ModCR) of EIRENE-internal COLRAD routines for H2 and D2, provision for T2 and DT.	12/2026
10.	Aalto-3	Assessment and validation of impact of D2 (versus H2) COLRAD for ion-molecular charge exchange using JET-ILW plasmas; if available, JT-60SA.	07/2027
11.	Aalto-4	Characterisation of impact of revised charge-exchange rates and photon opacity in ITER.	11/2027
12.	KUL-1	Technical implementation of fluid model for molecular species in SOLPS-ITER.	06/2026
	KUL-2	First implementation of extended KDMC model finished and benchmarks for validation and uptake in TSVV-B and C defined.	10/2026
12.	KUL-3	Integration fluid molecule model in SpH scheme. Merge request in SOLPS-ITER and EIRENE-NGM (FZJ "JuGit") repositories.	06/2027
	KUL-4	Performance and accuracy of KDMC model evaluated and benchmark requirements for uptake in TSVV-B and C reached.	10/2027

The milestone names indicate which of RUs (and respective team members) contribute mostly. The following chart indicate optimal time for potential code camps ("CC"), milestone version of EIRENE-NGM release ("MsV") and final report ("F.R"). It also puts the above tabulated milestones into the context of main development lines.



Scientific deliverables (up to 1 page)

The table below provides an overview of deliverables per WP. The deliverables are revised to fit into the 3 PPY. For possible extensions the reader is referred to the original proposal.

Year	Description
2026	**WP0: Overall project management and code maintenance** 1) Report on the detailed discussions with TSVV-B/C and ACHs regarding coupling and performance requirements for the associated codes as well as on EIRENE development progress (D.V. Borodin). **WP1: Model hierarchy and interfaces** 2) Report with governing equations for advanced fluid model for molecules, including transport coefficients and boundary conditions, and the description of coupling to fluid atom model and plasma equations (W. Van Uytven, W. Dekeyser) 3) Neptune with first implementation of KDMC and assessment of memory and performance gains w.r.t to full kinetic and AFN simulations. (Thijs Steel, G. Samaey) 4) First version of the STYX2.0 interface to EIRENE (joint work with TSVV-B) including all key features of STYX1.0 (Nicolas Rivals) 5) Version of STYX2.0 allowing to use coarser grids in EIRENE than in the fluid code. Demonstration of the advantages on the memory footprint and acceptable discretization errors. (Nicolas Rivals) 6) Report assessing the recycling time scales (molecular outgassing) observed in the stand-alone wall model using a stochastic model for turbulent fluxes, as a function of wall parameters (Julien Denis). **WP2: Collisional radiative models** 7) Provision of at least 3 datasets for ModCR (so also for PLOUTOS) including for hydrogen isotope containing molecules with resolution by vibrational states (optionally also rotational) for mixed species (Dmitriy V. Borodin, Francesco Cianfrani, Pieter W. Groen). 8) Report on the significance of isotope effects and qualification of the uncertainties including those due to the missing/inaccurate A&M data (Dmitriy V. Borodin, Francesco Cianfrani, Michael Gordon). 9) Report on ModCR (with PLOUTOS data) validation against other codes (e.g. Yacora) and experiments (JET, PSI-2).

	10) Release of consolidated version of standalone ModCR (Michael Gordon, Pieter W. Groen 11) Verified and validated collisional-radiative model in EIRENE (COLRAD subroutines) and photon opacity module in SOLPS-ITER (Mathias Groth, Ray Chandra, Timo Kiviniemi) 12) Report on characterisation and validation of impact of photon opacity against high-density divertor plasmas in JET-ILW using available measurements in UV and visible wavelength range measurements (Mathias Groth, Ray Chandra, Timo Kiviniemi).
2027	**WP0: Overall project management and code maintenance** 13) Report/overview paper on the code status and its interfaces and future development plans for usage in the other TSVV-codes. Release (D.V. Borodin) 14) Updated EIRENE version released through JuGit base repository and associated repositories at ITER and EUROfusion, including CI tests and updated webpage (D. Borodin, D. Harting, F. Cianfrani) **WP1: Model hierarchy and interfaces** 15) Report on validity and accuracy of enhanced AFN model through rigorous comparison with EIRENE, incl. D-T simulations and integration of new fluid models into SpH scheme (Wim Van Uytven, W.Dekeyser) 16) Tested and performance optimized KDMC version in Neptune (Thijs Steel, G.Samaey) 17) Report on implementation/verification of time dependent mode for reduced resolutions turbulence case (SOLEDGE3X-EIRENE), incl. corresponding STYX2.0 interface and documentation of proper parameter tuning (Nicolas Rivals) 18) Verified EIRENE module including time dependent recycling model (Julien Denis) 19) Technical demonstration of a 3D turbulent simulation of a medium size tokamak including full physics neutrals with SOLEDGE3X-EIRENE, leveraging the EIRENE OpenMP parallelization layer and grid decoupling (coarser grid for neutrals) in collaboration with TSVV-B (Yannick Marandet). **WP2 Collisional radiative models** 20) EIRENE release with consolidated MsV version of ModCR, including documentation (Michael Gordon, Pieter W. Groen, D.V. Borodin). 21) Publication on validation of the EIRENE version containing the new ModCR module (Dmitriy V. Borodin, Francesco Cianfrani) and demonstrating the new capabilities and performance. 22) Extended molecular database including T and D-T, and report on application with SOLPS-ITER to i) JET-ILW T and D-T, and ITER; ii) if available, utilise for JT-60SA H and D (Mathias Groth, Ray Chandra, Timo Kiviniemi).

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