TO: A. WINGEN
FROM: M.L. REINKE
SUBJECT: INITIAL GUIDANCE FOR EXAMINING OPTIONS FOR TOOLS TO CALCULATE HEAT FLUX TO 3D PFCS FOR R18-1/1-G1

<u>Background</u>
For the Recovery Project, NSTX-U has modified NSTX-U-RQMT-GRD-001, General Requirements Document (Section 4.1.1) so that the current and toroidal field directions are fixed. This opens up the possibility to use PFC designs that are non-axisymmetric, e.g. using 'fishscaling' or 'ski-ramping', so that for a given range of input angles, leading edge heat loads are eliminated. This is discussed more in Section 2.3 and 3.1 of the PFC System Requirements Document, NSTX-U-RQMT-SRD-003 and is presently envisioned for high heat flux, castelletd PFCs in the IBDV, IBDH and OBD R1/R2. Low heat flux regions may also have front-surface holes for fastener access and the outboard divertor is constructed from a series of faceted plates which can lead to heat flux enhancements, as discussed in PFCR-MEMO-005. Additionally, due to alignment uncertainties and the vertical growth of the centerstack, there is likely to be a poloidal 'step' moving from the IBDH to OBD surfaces. These all indicate a complex heat flux pattern that would originate from an asymmetric plasma due to non-axisymmetric material surfaces.

PFC design verification is being completed assuming simple heat loads defined by heat fluxes and purely toroidal angles of incidence, but there is a desire to commission scenarios that are supportable for the final as-built designs. As shown in the TSG scoping studies (PFCR-MEMO-008, -009, -010) at lower elongation and weaker poloidal flux expansion, NSTX-U can produce surface heat fluxes well above those anticipated to be supported by any PFC designs. Within the PFCR-WG, evolution of equilibrium generation tools will be completed (PFCR-MEMO-017) along with studies to interpret sub-surface temperature measurements (PFCR-MEMO-015). While existing tools such as W_PFC (PFCR-MEMO-004, -007) can generate heat loads from GEQDSK files for axisymmetric PFC contours, an investigation of how the plasma heat loads and perhaps limits fully 3D PFCs is warranted.

The goal of this activity is evaluate and demonstrate options to generate surface heat flux data using NSTX-U CAD models, GEQDSK equilibria and an estimate of the SOL heat flux profiles, e.g. the upstream midplane profile.

<u>Description of Options</u>
The need for this capability is not new within the magnetic confinement fusion community. PFCFlux has been used on JET, WEST and EAST and is an established tool developed and maintained by CEA. The CEA group, M. Firdaouss, has demonstrated an example of using PFCFlux on an NSTX-U equilibrium and geometry. This is available upon request, but is not a published

result. It is expected that PFCFlux would provide the needed capability, but there are questions if the speed of the code can service NSTX-U operational goals and an additional challenge of needing to establish an MoU and collaboration between CEA and PPPL. Evaluation may be possible through ORNL.

The SMARDDA/SMITER code has been developed by CCFE and used to compute heat fluxes on MAST-U and ITER. Evaluation of this code is possible through staff collaborating with JET/MAST-U as SMITER is installed on the Freia system. This has yet to be evaluated for an NSTX-U like case, but is planned.

A remaining option would be to extend existing ORNL tools such as DIV3D (see Appendix A) used in W7-X design work or build upon established field-line tracing codes used by ORNL on DIII-D.

Thus an important question to answer is whether to establish a local (PPPL-based) capability to generate heat flux on 3D PFCS by using an existing tool, or develop something new with the intention of establishing a new capability not supported by PFCFlux or SMITER. It is not desirable to create a new 3D heat flux modeling tool which simply duplicates an existing community capability.

Desired Criteria for Evaluating Options

The following is expected to be necessary to support this activity for NSTX-U:

- The ability to import a standard class of CAD output format(s): STEP, STL, IGES, etc. Note that NSTX-U designs are native to CREO.
- The ability to import equilibria from standard GEQDSK format.
- The ability to run double & near double null geometries and specify the power sharing separately between all four divertor regions.
- Ability to specify the heat flux profile to the PFCs with at least the capability to simply invoke an 'Eich' profile with a 'spreading factor – S' and upstream heat flux width, λ_q. See (1) and (2) in [Eich – PRL 2011]
- The ability to complete the computation of the heat flux pattern on a machine segment of $\geq 30^o$ toroidally for a single equilibrium in < 5 minutes, accounting for > 95% of the power using PPPL-like computing resources.
- Deployable and maintainable for computing systems similar to those available at PPPL: https://researchcomputing.pppl.gov/

To evaluate these capabilities, a GEQDSK file and the CAD geometry are available here. Additional CAD formats can be made available upon request. Simulations should assume 2.8 MW to each of the outer divertors and 0.7 MW to each of the inner divertors. A heat flux of width of λ_q=5 mm with a spread factor of $S = 1$ mm should be assumed, to match the already completed PFCFlux simulations.

Desired Enhanced Capabilities

The following would be desired as enhanced capabilities that might be feasible within future upgrades:

- The ability to complete the computation of the heat flux pattern on a machine segment of ≥ 30^{o} toroidally for a single equilibrium in < 1 minute, accounting for > 95% of the power using PPPL-like computing resources.
- The ability to specify a 2D (R,Z) axisymmetric emissivity profile and generate radiative heat flux to PFCs.
- The ability to utilize 3D equilibrium solutions, e.g. M3D-C^1 or EMC3-EIRENE output, that will allow for non-axisymmetic heat flux patterns on non-axisymmetric PFCs. This is motivated by the concern over intrinsic error fields due to inner PF coil alignment for NSTX-U.
- The ability to utilize equilibra with snowflake geometries.
- Deployable and scalable for leadership class computing systems similar to those available at ORNL (e.g. Summit, Titan).

Initial Execution Plan

The following work breakdown is planned:

- Reinke – demonstrate and evaluate the use of SMITER
- Wingen – demonstrate and evaluate a custom-built solution using existing field line tracing codes

A future PFCR-WG MEMO will report on the results of this investigation.

Appendix A – Description of DIV3D [J. Lore Private Communication 1/26/2018]

The code DIV3D [1,2] was developed to calculate heat loads to 3D plasma facing components (PFCs) for the Wendelstein 7-X stellarator, as part of the design of new divertor components. DIV3D approximates heat transport from the plasma core to the PFCs and allows for both the magnetic field description and the components to be three dimensional. The code initiates a large number of field lines on a closed flux surface and follows these fields lines with cross-field diffusion until a component is intersected. The diffusivity has the form $D_m = (\Delta_\perp)^2/\Delta_{||}$, where the distances $\Delta_\perp$ and $\Delta_{||}$ are step sizes perpendicular and parallel to a field line, respectively. This quantity can be approximately related to plasma physics parameters as $D_m \sim \chi/T^{1/2}$, where χ is the cross-field thermal diffusivity and T is a characteristic temperature. Given an initial energy weighting (e.g., isotropic or ballooning-like), the heat fluxes are calculated by summing the number of intersections multiplied by the energy and divided by the area. As the intersection points are stored, the resolution can be increased in postprocessing by remapping the points to a refined mesh. The code scales extremely well with the number of processors as each field line tracing is independent.

The code can be applied to calculate the fluxes to nonaxisymmetric components in NSTX-U, accounting for tile gaps and fishscaling. Some speed improvements can be expected, as the bounding shape (the toroidally averaged component surface) is known, which will simplify the checking for intersections. Additionally, the field line derivatives are inexpensive to calculate for axisymmetric magnetic fields as compared to 3D models. The code has already been generalized to use 3D magnetic field models from several equilibrium codes [3], which will facilitate the implementation of additional field models for NSTX-U, such as the vacuum approximation of accounting for 3D applied and error nonaxisymmetric fields, as well as full 3D equilibrium solutions. When designing the W7-X divertor components, DIV3D interfaced with CAD drawings through the use of STEP files with specially labeled points. This method can also be applied to NSTX-U drawings, allowing for rapid reevaluation of fluxes if the design evolves.

[1] J.D. Lore, T. Andreeva, J. Boscary, S. Bozhenkov, J. Geiger, J.H. Harris, et al., “Design and Analysis of Divertor Scraper Elements for the W7-X Stellarator,” IEEE TPS 42, 539 (2014).

[2] J. Lore, T. Andreeva, J. Boscary, J. M. Canik, J. Geiger, J. H. Harris, et al., “Heat flux and design calculations for the W7-X divertor scraper element,” in Proc. 24th IAEA Fusion Energy Conf., Oct. 2012, no. FTP/P1-02, pp. 013015-1–013015-15.

[3] J.D. Lore, M. Cianciosa, H. Frerichs, J. Geiger, H. Hoelbe, J. Boscary, and the W7-X team, “Modeling and Experimental Testing of Heat Fluxes on W7-X Divertor Scraper Elements”, IEEE TPS (2017, accepted)

Record of Changes

Rev.	Date	Description of Changes
0	3/23/2018	Initial release for review