1. Purpose of Experiments
Include immediate goal of the experiments, scientific importance and/or programmatic relevance. Refer to any relevant program milestones.

The immediate goal of this experiment is to quantify the amount of ammonia produced in Alcator C-Mod during N-seeded discharges. Experiments will be performed in both USN and LSN scenarios to investigate the impact of divertor geometry and cryo-pump location. This is of great interest to the ITER team in terms of tritium handling requirements since the ITER tritium recycling facility has assumed ammonia concentrations on the order of 1-10 appm in the exhaust stream. The concern arises since experiments on ASDEX-Upgrade [1] have shown as much as 8% of injected nitrogen is converted to ammonia. The T-plant in ITER is currently designed for low levels (ppm) of ammonia in the exhaust gas. In addition, the ITER cryo-pumps will use active charcoal, where tritiated ammonia can get adsorbed. To desorb ammonia, a high temperature regeneration of the cryo-pumps will be needed, and significant ammonia accumulation might impact the overall operation duty cycle. It is therefore important to characterize how, how much, and where ammonia is formed in a fusion device.

2. Background
Discuss Physics Basis of the proposed research. Prior results at Alcator or elsewhere, and any related work being carried out separately.

Impurity seeding is needed for radiative dissipation and heat flux mitigation on PFCs in high-power divertors. Nitrogen is a leading candidate for edge-seeding as it allows for substantial heat flux mitigation while maintaining high core confinement. However, nitrogen also introduces chemistry into the system as it is chemically active with hydrogenic species. Plasma-assisted ammonia (NH$_3$) formation is a well-documented phenomenon in the low-temperature plasma physics community [2,3]. This process is
further complicated by a wide range of surface chemistry [4-6] and catalyst effects [2], which may or may not play a role at high plasma fluxes [7].

Work in ASDEX-Upgrade [1] and JET [8,9] both indicated ammonia production from nitrogen-seeded plasmas in metal machines. The ASDEX-Upgrade results were measured during and post-discharge via Residual Gas Analysis (RGA) with quantification through careful calibration of the RGA systems as well as theoretical treatments and interpretations of the cracking patterns to distinguish the NQ$_3$ signal from the Q$_2$O and CQ$_4$ signals and components. The conclusion from the ASDEX-Upgrade results is that ~8% of the injected nitrogen is recovered as ammonia in the exhaust gas. The JET results are more qualitative but clearly show the presence of ammonia from the cryopump regen of the LN2 panels [3]. The JET results also show nicely how the use of $^{15}$N for seeding allows the $^{15}$ND$_3$ peak (mass 21) to be differentiated from the common and often strong D$_2$O peak (mass 20). This is something that should be considered for this proposal as well for ease and accuracy of quantification of the ammonia production rate.

![Figure 1: Comparison of m20 and m21 signals from JET cryo-pump regen [3]. A comparison between partial pressures of m20 and m21 is considered to be an effective way to distinguish ammonia from other species populating m20.](attachment:figure1.png)

This proposal is part of a coordinated effort driven by ITER request to measure ammonia formation in metal machines to get a more accurate picture of expected ammonia formation in ITER. It is high priority and urgent since the results will drive and motivate potential design changes in the ITER tritium handling facility. C-Mod’s key contributions to this effort are that it is a full metal machine with no history of carbon usage (i.e. lower interfering residual hydrocarbon signals), it can form ITER-like edge plasmas where the ammonia formation is likely to be driven, and it has the ability to operate in both closed (LSN) and open (USN) divertor geometries to investigate any dependence of ammonia content on divertor geometry.
3. Approach

Describe the methodology to be employed; explain the rationale for the choice of parameters, etc. Describe the analysis techniques to be employed in interpreting the data, if applicable. If the approach is standard or otherwise self-evident, this section may be absorbed into the Experimental Plan.

The concept of the experiment is similar to Bruce Lipschultz’s gas balance experiments. We want to inventory a gas species pumped (Ammonia) and relate it to the amount of gas initially injected (Nitrogen). However, the key difference is that the pumped gas will not be measured via pressure change or solely via RGA after the discharge, but rather the pumped gas will be “collected” on the cryopump and inventoried and quantified during a LN$_2$ panel regen on the cryo pump after the experiment.

The produced ammonia will condense on the LN$_2$ panel of the cryo pump which means that the cryo pump LHe panel can still be regenerated in between discharges without worrying about releasing some of the produced ammonia as well (although the RGA should be monitoring for such an event).

The seeded gas to be used is $^{15}$N$_2$, which is readily available for reasonable price in the quantities needed for this experimental plan (e.g. $230 for 175$ torr-L, $375 for 350$ torr-L). The shot scenario this MP is based on (shot #1091019023) used ~10 torr-L of N$_2$ for seeding. The advantage of using $^{15}$N for seeding is that deuterated-ammonia formed will appear at mass 21 on the RGA, which is distinct from the signal from D$_2$O at mass 20, which is expected to be the major background signal. While this may make the qualitative ammonia production data cleaner, it also makes quantification more expensive as $^{15}$ND$_3$ (e.g. $930 for 1000$ torr-L) will be needed for RGA calibration.

The proposed plan is for two half-day experiments. A half-day is required such that several simultaneous shots can be performed to build up ammonia inventory in the cryopump to assure a strong signal for analysis from the RGA during the cryo regen. Following the $^{15}$N-seeded shots, several non-seeded shots are needed to “complete” the ammonia production as was shown in ASDEX-Upgrade [1].

![Figure 2: The sequence of N$_2$ seeded and non-seeded discharges in ASDEX-Upgrade [1] demonstrating that significant ammonia production continues after seeded discharges.](image)
It is not entirely clear why ammonia production continues despite no new nitrogen being seeded but it is suspected (by us) it may have to do with nitrogen adsorption on the wall continuing to react and form radicals during subsequent discharges. It is thus hard to predict how ammonia production in non-seeded discharges will compare as to what is seen in ASDEX-Upgrade where the shot duration is much longer (~8 s) but the densities and heat fluxes are typically lower. It is suggested here for 4-5 non-seeded discharges to complete the ammonia production in C-Mod to compensate for the shorter pulse length if that is an issue. This is why it is thought a half-day at a minimum is required for each of our proposed two scenarios (LSN and USN).

Those scenarios are running similar discharges in both LSN and USN to compare the ammonia production between the two geometries. The concept of using both LSN and USN discharges is to test the impact of divertor geometry and cryo-pump location on the resulting ammonia production. Ammonia is a “sticky” molecule, thus it stands to reason that production from a closed divertor may result in a significantly higher fraction of the produced ND₃ to attach to the wall rather than be carried out in the neutral exhaust gas. This is important in determining how to extrapolate results on devices with more open divertors (e.g. JET) to the closed divertor of ITER. However, the cryo-pump in C-Mod is located at the top of the machine so a USN discharge is also a closer reconstruction of the cryo-pump location in ITER with respect to the divertor.

The baseline shot scenario proposed for this work is shot# 1091019023, which is Alberto Loarte’s trophy shot from his work with nitrogen-seeded high performance discharges for ITER. Since this is work directly related to ITER it seems appropriate to have the plasma conditions as ITER-like as possible. This shot is a LSN discharge but similar edge plasma parameters would be desired for the USN scenario as well.

During the discharge, spectroscopy can be used to monitor for ND-radicals, which can hopefully reveal some information on where the ammonia formation is taking place and also qualitative data during the discharge. If AIMS is available it might also be able to track where the ¹⁵N ends up in the walls. After the discharge with the gate valves still closed, the RGA can sample the chamber through the by-pass valve to monitor the presence of ammonia as a function of time, and can continue to monitor once the gate valves are opened and the LHe panel on the cryo-pump is regenerated in between discharges. At the end of the day, the RGA will monitor the relevant mass signals as the cryo-pump LN2 panels are regenerated up to room temperature. Integrating these signals with the calibration from a controlled puff of ¹⁵ND₃ into the C-Mod vessel will allow us to quantify the total ammonia production and compare this to the total amount of ¹⁵N₂ injected.

A table summarizing requirements and their respective approaches is below:

<table>
<thead>
<tr>
<th>Requirement</th>
<th>Approach</th>
</tr>
</thead>
<tbody>
<tr>
<td>Gas balance measurement</td>
<td>Gate valves closed during discharge</td>
</tr>
<tr>
<td></td>
<td>Cryopump only</td>
</tr>
<tr>
<td></td>
<td>Gate valves open for cryo LHe panel regen in between</td>
</tr>
</tbody>
</table>
shots
- RGA running post-discharge via by-pass valve and during cryo LHe panel regen
- Full regen of cryo at end of day with RGA to monitor recovered gas species

RGA Calibration
- Loading of custom gas (\(^{15}\text{ND}_3\)) into plenum for injection and RGA measurement during “blank” shot

Minimize contributing signals
- No nitrogen seeded work since the last full cryo regen
- Preferably fully regen the cryo the day before to minimize “initial inventory” and background signals
- Use \(^{15}\text{N}\) for impurity seeding

4. Resources

4.1 Machine and Plasma Parameters

Give values or range for:

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Toroidal Field</td>
<td>5.4 T</td>
</tr>
<tr>
<td>Plasma Current</td>
<td>0.8 MA</td>
</tr>
<tr>
<td>Working Gas Species</td>
<td>Deuterium</td>
</tr>
<tr>
<td>Density</td>
<td>(n_0 = 1.5 \times 10^{20} \text{ m}^{-2})</td>
</tr>
<tr>
<td>Boronization Requested</td>
<td>NO for 2 half days, YES (within 2 experimental days) for 1 half day</td>
</tr>
<tr>
<td>Equilibrium configuration</td>
<td>LSN (\rightarrow) similar to 1091019023, USN (\rightarrow) parameters similar to 1091019023</td>
</tr>
</tbody>
</table>

4.2 Auxiliary Systems

<table>
<thead>
<tr>
<th>System</th>
<th>Setting</th>
</tr>
</thead>
<tbody>
<tr>
<td>ICRF Power, pulse length, phasing</td>
<td>3 MW at 0.6 s, ramping to 4 MW at 0.8 s, ramping to 4.5 MW at 1.5 s then off</td>
</tr>
<tr>
<td>LHCD Power, pulse length, phasing</td>
<td>N/A</td>
</tr>
<tr>
<td>Pellet Injection (species)</td>
<td>No</td>
</tr>
<tr>
<td>Impurity blow-off injection</td>
<td>No</td>
</tr>
<tr>
<td>Diagnostic Neutral Beam</td>
<td>No</td>
</tr>
<tr>
<td>Special gas puffing</td>
<td>Yes, (^{15}\text{N}) seeding, custom gas mixture for calibration of RGA</td>
</tr>
<tr>
<td>Cryopump</td>
<td>Yes with full regen at end of day</td>
</tr>
<tr>
<td>Non-axisymmetric Coils (Connections, Current)</td>
<td>No 00</td>
</tr>
</tbody>
</table>

4.3 Diagnostics

List required diagnostics, and any special setup or configuration, e.g. non-standard digitization rate.

Emission spectroscopy (ND+, N, D), Langmuir probes, RGA, Divertor IR imaging
AIMS (if available)

5. Experimental Plan

June 5, 2015
Both sections must be filled in.

5.1 Run sequence Plan
Specify total number of runs required, and any special requirements, such as consecutive days, no Monday runs, extended run period – 10 hours maximum – etc.

Since materials/surfaces can be catalysts for ammonia production and there are no plans for boron in ITER, in order to make this experiment as ITER-like as possible, it is best not performed recently after a boronization. We would like to work with metal walls as clean as possible. Comparison of these results with ammonia production after a recent boronization would also allow us to determine if the wall surfaces are acting as significant catalysts in ammonia production.

We are requesting three half days with the half day preferably in the later half of the day so following experiments won’t impact results prior to the cryo-pump regeneration. It is also preferable if experiments in the first half of the day do not have any nitrogen seeding planned. LSN discharges will need to occur during forward-field operations and USN discharges will require reverse-field operation.

Discharges will be pumped by the cryo only (turbo gate valves closed) with only the bypass valve to the RGA open so the chamber can be sampled while the produced ammonia and other residual gases are pumped by the cryo. After an appropriate amount of time (5-7 minutes?) the gate valves will be opened so the LHe panel of the cryo can be regenerated in between shots (similar to Bruce Lipschultz’s gas balance experiments).

We would like for there to be a LN$_2$ cryo regen the day before the experiment so that stored inventory (i.e. potential background signals) in the cryo is minimized. Then the cryo will be regenerated at the end of the day as well to quantify the total ammonia production for the experiment. We are willing to monitor the regens and RGA but this may require after-hours engineering support if necessary.

5.2 Shot sequence plan
For each run day, give detailed specification for proposed shot sequence: number of shots at each condition, specific parameters and auxiliary systems requirements, etc. Include contingency plans, if appropriate.

Half-day 1 (LSN, forward field, no boronization):

Shot 1-3: $^{15}$N-seeded LSN discharges (similar to shot 1091019023)

Shot 4-end: Repeated shots with no seeding to complete/saturate formation of ammonium. Plasma parameters may need to be reduced to prevent excessive perpendicular heat flux to PFC surfaces. Neon seeding may also be an option.

Half-day 2 (USN, reverse field, no boronization):

Shot 1-3: $^{15}$N-seeded USN discharges (USN version of 1091019023?)
Shot 4-end: Repeated shots with no seeding to complete/saturate formation of ammonium. Plasma parameters may need to be reduced to prevent excessive perpendicular heat flux to PFC surfaces. Neon seeding may also be an option.

Half-day 3 (LSN, forward field, recent boronization):

Shot 1-3: $^{15}$N-seeded LSN discharges (similar to shot 1091019023)

Shot 4-end: Repeated shots with no seeding to complete/saturate formation of ammonium. Plasma parameters may need to be reduced to prevent excessive perpendicular heat flux to PFC surfaces. Neon seeding may also be an option.

6. Anticipated Results
Discuss possible experimental outcomes and implications. Indicate if the program may be expected to lead to publications, milestone completions, improved operating techniques, etc. Indicate if the experiments are intended to contribute to a joint research effort, an ITER request, or an external database.

This experiment is proposed at the request of the ITER organization since it has significant potential to reveal design implications, specifically for the tritium handling plant, and thus they are high priority and urgent.

There will certainly be ammonia formed but due to the complex nature of plasma-assisted ammonia production and the influence of surface conditions and surface chemistry it is impossible to predict if it will be greater or less than the 8% conversion rate measured in ASDEX-Upgrade [1]. It is also currently unclear where the ammonia formation actually takes place inside the device. This uncertainty is why these experiments are so critically important to ITER and why the ITER-like SOL plasmas in C-Mod make them so relevant.

If an ammonia conversion factor can be measured with even first order accuracy this is a publishable result. Not only is this relevant for ITER but it is important in understanding safety implications and the tritium cycle for any device running tritium with nitrogen seeding. The quantification of the results is also likely to be more straight-forward in the all-metal environment of C-Mod since interference from hydrocarbons (e.g. methane) will be less of an issue, which may lead to a more reliable and accurate quantification than is achievable on other devices. The comparison of the divertor geometries and impact of the wall composition will also give this work an aspect that has previously been overlooked.

7. References
Include references both to external and internal literature or communications, which bear on this proposal. See Section 2.