FINDINGS
OF THE
ORGANIC CONTAMINANTS SCIENCE
STEERING GROUP (OCSSG)

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Note: This is the presentation version of the white paper “Report of the Organic Contamination Science
Steering Group”. If there are any discrepancies between the two documents, the white paper should be
judged to be superior.
OCSSG Charter

The Organic Contaminants Science Steering Group was charted through MEPAG to analyze three questions:

1. **Problem Definition.** What is the best way to define the issues regarding the impact of organic contaminants on future lab-related scientific investigations at Mars? (We need to define the problems clearly before we can mount a serious attempt to solve them).

2. **Problem Priority.** What is the degree of importance the science community assigns to the issues defined above in #1?

3. **Approach to Problem Solution.** Recommend an approach to resolving any defined, high-priority problems.
Problem Definition

Problem #1
We need to establish a definition of “clean” that applies to molecular organic contaminants, taking into consideration their expected detection limits by various missions. This is a prerequisite to systematic application of the general methods of molecular biology at Mars.

Solution
We propose the structure of a new definition of “clean”, which is from the perspective of the sample as it is delivered to the instruments, rather than from the perspective of spacecraft surfaces.

- For the science community this definition is simple and gets to the heart of the matter.
- However, for spacecraft engineers, the approach is non-traditional.
Problem Definition

Problem #2

We do not have a scientific consensus on the organic contaminants of importance to in-situ lab instruments in general, their general relative priority, and agreement on concentration levels that are achievable by the spacecraft engineers and useful to the instrument PIs.

Note: Each PI can form his/her own judgement on contaminant priorities. However, what has been missing is the development of a community-based consensus which can be used in a pre-competitive environment.

Solution

- An interim consensus solution is presented in this study.
Problem Definition

Problem #3

In order to achieve definitive scientific results in an in-situ sample analysis mission, it is necessary to be able to distinguish contaminants from natural signal. For organic molecular contaminants, the design of the procedures necessary to achieve this have not been established.

Solution

The OCSSG offers several possible approaches (in priority order) to mission design teams and to the science community. These solutions range from definitive to helpful. OCSSG defers to the future mission science/engineering teams to select an approach that is most appropriate for their circumstances.
Problem Definition

Problem #4

For NASA's missions that are planning measurements of in-situ organic geochemistry (including Phoenix, MSL, and future), there has not yet been enough planning on how to achieve an initially clean sample system AND to maintain its cleanliness throughout all measurement operations.

Solution

The OCSSG offers several possible approaches to mission design teams and the science community. OCSSG defers to the future mission science/engineering teams to select an approach that is best for them.
Problem Priority

The four problems described above are of very high priority to the Mars exploration science community. For astrobiology-related landers, these issues can lie at the heart of their science logic, and can make the difference between the eventual results being definitive, or merely being suggestive.
Starting Assertions
Nature of contaminants and priority

1. For the scientific objectives of missions with an in-situ lab, the primary contaminant issue is the quantity of organic contaminants which will transfer to a sample on its way to a detector. The portion of the contaminant load which does not transfer to the samples is, for this kind of experiment, irrelevant.

2. Earth-sourced and Mars-sourced contaminants need to be considered separately.
   - Until organic carbon is definitively discovered on Mars, preventing ANY sample from receiving Earth-sourced organic contaminants above the level of detection is the highest priority.
   - Once Mars-sourced organic material has been proved, minimizing cross-contamination of Mars-sourced organic material between samples, so that its variation can be studied, will become critical.
   - Both issues MAY become relevant for the same mission (most notably, MSL).
Approach to Solution
Definition of "Clean"

Traditional Definition
Contamination control engineers traditionally define clean from the perspective of spacecraft surfaces.

Proposed New Approach
Definition: A clean sample (or sample split) is one which has been delivered to an instrument with less than a specified amount of contaminants.

- Will require a further specification of the amount and nature of allowable contaminants (which will likely differ for each mission). We recommend the specification be by mass fraction (i.e. ppb).
- This definition incorporates the concept of transferability, which distinguishes potential from actual contaminants.
- Requires understanding the overall system-level performance of the sample system.

Note: The particulate surface cleanliness is a unitless value that incorporates size bin and number of particles per unit surface area based on an analytical slope. The specifics are stated in IEST-STD-CC1246D

<table>
<thead>
<tr>
<th>Cleanliness Level</th>
<th>1</th>
<th>2</th>
<th>3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Non-volatile residue (NVR) (nanograms/cm²)</td>
<td>500</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>Particulate cleanliness level</td>
<td>400</td>
<td>200</td>
<td>25</td>
</tr>
</tbody>
</table>
Approach to Solution

Proposed General Hierarchy of "Clean" Requirements

We advocate the following requirements hierarchy.

**Primary Requirement**

1. TBD mission shall have the capability to acquire and deliver clean samples of martian materials to its instruments.

**Derived Requirements (examples only)**

1. Design.
   - Minimize the use of organic materials within the sealed volume.

2. Spacecraft manufacture, assembly.
   - The general surfaces shall meet or exceed Cleanliness Level 1.
   - The general sample acquisition and processing facility surfaces shall meet or exceed Cleanliness Level 2.
   - The spacecraft surfaces that will come in direct contact with samples shall meet or exceed Cleanliness Level 3.

3. Operations
   - Keep the clean parts of the system warm.
   - Flush the system with a cleansing sample prior to collecting data.
Approach to Solution
"Clean" Definition and Timing

The degree of specificity of the "clean" definition for each mission may depend on the timing.

Pre-competitive Environment

In a pre-competitive environment, it is important that a flight project commit to a certain promised state of sample cleanliness in advance of its instrument competition.

- The ability of the instruments to make use of the specified level of cleanliness may become a selection criterion, and thus must be known in advance.
- The nature of the allowable concentrations of contaminants needs to be general enough to allow for meaningful competition.

Post-competitive Environment

In a post-competitive environment, each flight project will negotiate with its selected investigators, consistent with any pre-competitive agreements, to define mutually acceptable contamination specifics.
Approach to Solution
Initial Priorities on Contaminants of General Interest

Of a very wide range of potential molecular contaminants considered by this SSG, the following were judged to be the biggest “worry” to the Mars exploration science community (not listed in priority order).

- Benzene and more complex aromatics
- Organic molecules with carbonyl or hydroxyl groups.
- Non-aromatic hydrocarbons
- Amino acids, amines, amides
- DNA

Concentrations

A general guideline is that samples need to be clean with respect to these contaminants at approximately the 1-10 ppb level. These values will be different for different missions. A specific recommendation for MSL is presented in Slide #18.
Approach to Solution
Distinguishing Contaminants from Natural Signal

In order for the data from a lander's organic chemistry lab to be interpreted correctly, the state of contamination of the sample system at the time of the measurement needs to be known. Possible strategies (in priority order):

NECESSARY TO ADDRESS POTENTIAL AMBIGUITY

1. Carry several splits of at least one standard of known "zero" composition in a form and position that they can be introduced as far upstream as possible into the sample chain.
   • The nature of the standard(s) needs more discussion—this should be worked with the PSG, once it is formed.

2. Before launch, contaminants should be measured both by the mission instruments where feasible AND by terrestrial instruments with higher sensitivity.

3. Collect witness plates during ATLO, and archive for later analysis.

EXTREMELY VALUABLE

1. Construct a duplicate of the critical sample/analysis systems, which can be held in pristine state (on Earth), and on which tests can be made during mission operations.
Approach to Solution
Mitigation and contamination control strategies

Establishing a clean surface.

1. In general, establishing an initially clean surface can be done through a combination of precleaning wipes, a series of solvent washes, and vacuum bakeout.

2. We need to validate that current methods to clean the contaminants of specific mission interest are sufficient.

The following ideas are suggested to engineering design teams.

1. Hardware should be “designed to clean”, modular and robust enough to be compatible with standard cleaning facilities.
   - Select fabrication materials for demonstrated cleanability.
Approach to Solution
Mitigation and contamination control strategies

Monitoring changes in the contamination state.

During the interval between cleaning and sample analysis at Mars, the state of contamination can change, and it must be monitored. The following are suggestions:

1. Pre-launch monitoring consisting of residual analysis of constituent species and their amounts through hardware closeout.

2. Post-launch contamination monitors (e.g. QCM, calorimeter) which operate in space during flight de-contamination cycles and on Martian surface prior to sampling.

3. Flight experiments use of controlled data.
**Approach to Solution**

**Mitigation and contamination control strategies**

**Maintaining a clean surface.**

Maintaining the cleanliness of a surface can be done by controlling the movement of molecular contaminants in the sensitive parts of the system after cleaning. The following design ideas are offered for engineering teams to use as appropriate.

1. Seal and pressurize the sample contact hardware after cleaning. It must specifically be isolated during cruise.

2. Keep the internal surface area and the total volume as small as possible. *(This one is really important!!)*

3. Minimize, or eliminate, the use of organic materials, and lubricants, within the sealed volume.

4. Design in and install getters sensitive to the contaminants of interest.
Approach to Solution
Mitigation and contamination control strategies

Maintaining a clean surface (cont.).

5. Minimize the size of the opening into the most sensitive areas.

6. Keep the temperature of the clean parts of the system higher than that of the surrounding sources of contaminants.

7. Use a vapor proof biobarrier that can be temporarily removed to protect the most sensitive portions of the clean system.

8. Include the capability to bake out the system either during cruise or on Mars.

9. Prior to running unknown samples, send a synthetic sample through the system which has getter properties with respect to the contaminants of interest.
Possible MSL Requirements

1. MSL shall have the capability to acquire, prepare, and deliver to its instruments clean samples of martian geologic materials that meet the contamination levels described in Table 1, through a combination of contamination control, system design, and operational procedure.

<table>
<thead>
<tr>
<th></th>
<th>Earth-sourced</th>
<th>Mars-sourced</th>
</tr>
</thead>
<tbody>
<tr>
<td>Total Organic Contaminants</td>
<td>40</td>
<td>not specified</td>
</tr>
<tr>
<td>Benzene or aromatic hydrocarbons</td>
<td>8</td>
<td>not specified</td>
</tr>
<tr>
<td>Carboxyl and hydroxyl containing compounds</td>
<td>10</td>
<td>not specified</td>
</tr>
<tr>
<td>non-aromatic hydrocarbons</td>
<td>8</td>
<td>not specified</td>
</tr>
<tr>
<td>amino acids</td>
<td>1</td>
<td>not specified</td>
</tr>
<tr>
<td>amines, amides</td>
<td>2</td>
<td>not specified</td>
</tr>
<tr>
<td>DNA</td>
<td>1</td>
<td>not specified</td>
</tr>
</tbody>
</table>

2. MSL shall implement procedures that will allow any organic detection to distinguish a terrestrial contaminant from a martian source.
Technology Development

Recommendations for the Mars Technology Program

1. Technology for biobarriers that are effective against molecular contaminants is judged to be insufficient.

2. We have insufficient knowledge on contaminant transferability, which is necessary to predict the system performance called for in our overall definition of "clean".

3. The state of the art in measuring the level of general residual molecular organic contamination (on Earth) appears to be sufficient without new basic technology development. However it is expected that the methodologies for assaying certain specific compounds will need to be improved (e.g. benzene, amino acids, nucleic acids (DNA and RNA)). These assay methodologies will need to be "ATLO-friendly".

4. We need new technologies for sterilization and the monitoring of efficiency and effects of sterilisation procedures on spacecraft materials.
External Validation

In addition to the discussions internal to this multi-disciplinary Science Steering Group, our initial conclusions were discussed at the 3rd European Exo/Astrobiology meeting (Nov. 17-19, 2003), which was attended by 260 astrobiologists. Our interim conclusions were refined based on feedback received from this broader community.

- Multiple requests for our white paper in progress—very significant interest in this topic by the community.