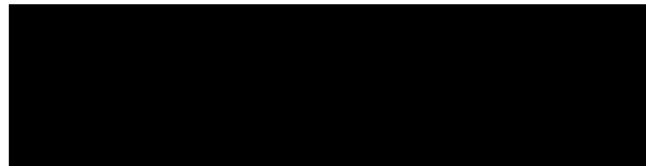


Advanced Exploration Systems Life Support Systems

Sabatier Catalyst Development

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NASA's Exploration Projects and Integration Office



INTRODUCTION:

The Exploration Projects and Integration Office at NASA Marshall Space Flight Center is interested in the development of a batch of Sabatier catalyst. Sabatier reactor catalyst converts metabolic carbon dioxide (CO_2) and hydrogen (H_2) to methane (CH_4) and water. Previous work regarding trace contaminants onboard the International Space Station (ISS) identified that gas contaminants that fouled the Sabatier reactor catalyst possessed poisonous chemical elements such as sulfur (S), silicon (Si), fluorine (F), and carbon (C).

The initial catalyst was developed by a third-party company. NASA seeks development of a similar baseline catalyst for internal contamination testing, and development of future solutions that will prevent catalyst bed poisoning.

GOALS AND OBJECTIVES:

As the Customer, NASA's Exploration Projects and Integration Office's objective is to provide funding to a Company (Vendor) to develop, synthesize, and produce a batch of Sabatier catalyst formulation informed by oversight and specifications provided by NASA's selected Technical Authority Consultant. Additionally, NASA requests the formulation batch synthesis data, chemical formulation, quality assurance and validation test data, and synthesis procedures are provided as a deliverable.

Performance Requirements and Deliverables:

The Vendor shall complete the following tasks:

Task 1: Synthesize a batch volume of 500 cubic centimeters (cc) of Sabatier catalyst. This will be referred to as the "baseline" Sabatier formulation. 400 cc of the baseline catalyst will be delivered to NASA. 100cc of catalyst will be used in comparative testing of alternate formulations as defined in Task 2. NASA is in possession of Ruthenium (III) Chloride catalyst precursor obtained through cancellation of prior work. NASA will transfer this chemical precursor to The Company and The Company will transfer the unused catalyst precursor to Marshall Space Flight Center after the contracted work is completed.

- The baseline catalyst formulation and synthesis will be documented, overseen, and advised by NASA NESC Technical Authority Consultant
- Determine approximate light off temperatures at residence times of 0.7, 1.0, and 1.5 seconds for molar ratios (MR) of H_2/CO_2 of 3.5, 4.0, and 4.5. Repeat each test 2 times. Each test should run for a minimum of 15 minutes once thermal equilibrium is achieved as indicated by appropriate placed thermal couples. Document product compositions once equilibrium is established. Total # of tests = 18.
- For references purposes, it is recommended that ICES publication AIAA 2013-3528 be used in reactor sizing and test configuration as this will allow for direct comparison to a similar test program for the existing ISS Sabatier flight catalyst. The previous test was conducted at 0.7 second residence time and a MR of 3.5. The reactor configuration in this previous testing used a diameter of 2.3 cm, length of 12.9 cm and a linear velocity of 16.8 cm/sec.

Task 2: Perform a literature search to identify a minimum of 3 alternate catalyst formulations for comparison to the baseline catalyst. It is initially recommended that one of these alternate formulations be nickel based, and the second and third formulations are to be determined based on the results of the

literature search with a specific emphasis on enhanced poison resistance against the compounds mentioned above in the introduction. It is understood that the number of combinations of active metal and support are almost infinite, and it is expected that at least 5 (or more) potential combinations will be provided and initially down selected to 3, as discussed above, after discussions with NASA.

Task 3: Produce approximately 50cc of the selected catalysts from task 2 and determine light off temperature at a residence time of 1 second and MR of H₂/CO₂ of 4.0. Repeat the test a minimum of 2 times and report product composition after thermal steady state is established for at least 15 minutes. Number of tests = 2.

Task 4: Identify and procure 1-2 samples of commercially available methanation catalysts and determine light off temperature and product composition in accordance with Task 3. Number of tests =2-4.

Task 5: Develop a Catalyst Data Package (CDP) containing catalyst batch synthesis data, chemical formulation data, quality assurance data which validates the product purity and metal concentration, and synthesis procedures.

Task 6: Conduct poisoning tests on the baseline catalyst and 1-2 additional catalysts to be collaboratively down selected from the identified poison resistant catalysts (Task 2) and commercial catalysts (Task 4). All 6 contaminants shall be introduced simultaneously. To provide for some level of historical comparison (aforementioned ICES paper) to the baseline ISS Sabatier catalyst, the residence time, linear velocity, and MR shall be 0.7 sec, 16.8 cm/sec, and 3.5, respectively. Contaminant concentrations are listed below in Table 1. For each test, establish equilibrium conditions for a minimum of 15 minutes prior to the introduction of the contaminants.

- Contaminant testing shall be conducted at the baseline nominal concentrations listed in Table 1 for a minimum of 300 hours, unless a significant reduction in catalyst activity is observed before the 300 hours are completed. Product concentrations shall be measured at a minimum of daily intervals.
- If no observable degradation is noted at 300 hours, the contaminant concentrations listed in Table 1 shall be increased by 10X. Testing shall then be continued for another 300 hours.
- If no measurable degradation in catalyst activity is observed after increasing the contaminant concentrations 10x for 300 hours, NASA and Reaction Systems will jointly define next steps.
- For estimating purposes, assume 3 catalysts shall be tested, for a total of 600 hours each.
- Develop a Test Data Package (TDP) for the poisoning tests containing the data and results from each of the poisoning tests.

Technical Specifications and Requirements:

Baseline catalyst – the baseline catalyst shall be produced using ruthenium chloride and TBD CPN alumina to produce an approximate TBD by weight Ru/Al₂O₃ catalyst. Final formulation specifics shall be defined collaboratively with NASA. For estimating purposes assume a final weight percent of ruthenium , based on the total catalyst weight, of 20%.

Specific methods of catalyst manufacturing of the baseline catalyst will be defined in collaboration with the NASA.

The catalyst shall be evaluated under the following conditions. Catalyst Test parameters are provided in Table 1.

Table 1: Parameter Table

Parameter	Value [units]
Hydrogen to Carbon Dioxide Molar Ratio ($\text{H}_2:\text{CO}_2$)	3.5:1
Carbon Dioxide flowrate	3.29 [SLPM]
Operating Pressure	14.7 [psia]
Concentrations of DMSO_2 (poison is sulfur) Molecular Weight = 94.13 g/mol ** Alternative dosing chemicals must stoichiometrically account for sulfur presence.	1.10 [mg/m^3] 0.28 [ppm]
Concentrations of DMSD (poison is silicon) Molecular Weight = 92.17 g/mol ** Alternative dosing chemicals must stoichiometrically account for silicon presence.	0.08 [mg/m^3] 0.02 [ppm]
Concentrations of Isobutane (poison is carbon) Molecular Weight = 58.12 g/mol ** Alternative dosing chemicals must stoichiometrically account for carbon presence.	5.82 [mg/m^3] 2.45 [ppm]
Concentrations of CS_2 (poison is sulfur) Molecular Weight = 76.13 g/mol ** Alternative dosing chemicals must stoichiometrically account for sulfur presence.	0.63 [mg/m^3] 0.20 [ppm]
Concentrations of COS (poison is sulfur) Molecular Weight = 60.07 g/mol ** Alternative dosing chemicals must stoichiometrically account for sulfur presence.	0.05 [mg/m^3] 0.02 [ppm]
Concentrations of R-218 Freon (poison is fluorine) Molecular Weight = 188.02 g/mol ** Alternative dosing chemicals must stoichiometrically account for fluorine presence.	1008 [mg/m^3] 131.10 [ppm]