

OFFICE OF THE DIRECTOR OF NATIONAL INTELLIGENCE



MAEGLIN (Molecular Analyzer for Efficient Gas-phase Low-power INterrogation)



Office of Smart Collection

Proposer's Day Brief – Kristy DeWitt

12 January 2016



Agenda

Time	Topic	Speaker
9:00am – 9:30am	Logistics, Program Introduction	Dr. Kristy DeWitt Program Manager
9:30am – 9:50am	IARPA Overview	Dr. Jason Matheny IARPA Director
9:50am – 10:10 am	Smart Collection Overview	Dr. Chris Reed Acting SC Office Director
10:10am – 10:20am	Break	
10:20am – 11:00am	MAEGLIN Technical Overview	Dr. Kristy DeWitt Program Manager
11:00am – 11:30am	MAEGLIN BAA Overview	Dr. Kristy Dewitt Program Manager
11:30am-12:00pm	Doing Business with IARPA	IARPA Acquisitions
12:00pm-12:30pm	Q&A Session	
12:30pm – 1:00pm	Lunch – on your own	
1:00pm – 3:00pm	Poster Session and Teaming Discussions	Attendees (No Government)



Disclaimer

- This Proposers' Day Conference is provided solely for information and planning purposes.
- The Proposers' Day Conference does not constitute a formal solicitation for proposals or proposal abstracts.
- Nothing said at Proposers' Day changes the requirements set forth in a Broad Agency Announcement (BAA).



Proposer's Day Goals

- Familiarize participants with IARPA's interest in research in low power, high sensitivity chemical detection.
- Familiarize participants with IARPA's mission and how to do business with IARPA.
- Provide answers to participants' questions.
 - This is your chance to alter the course of events.
- Foster discussion of synergistic capabilities among potential program participants, i.e., facilitate teaming.
 - Take a chance – someone might have a missing piece of your puzzle.



Important Points

- Proposer's Day slides will be posted on iarpa.gov
- Please save questions for the end, write on notecards
- Posters are available for browsing during break/lunch
- Government will not be present during the poster/teaming session
- Discussions with PM allowed until BAA release
 - Once BAA is published, questions can only be submitted and answered in writing via the BAA guidance.
- Name/email list of Proposer's Day participants provided to the group **with permission**



MAEGLIN Program Introduction



What's in a Name?

- In Tolkien's mythology, Gondolin was the great mountain-ringed city of the elves which remained hidden and safe for nearly 500 years. Its location was betrayed by Maeglin, out of spite after he was forbidden from marrying the king's daughter. Gondolin was then attacked by surprise and destroyed in a night.
- The **MAEGLIN Program** will provide a new method for discovering chemical fingerprints which currently remain hidden...



The Problem:

Positive ID of Complex Chemical Mixtures

State of the Art

- Contact, close range, or dog screening
- In all cases → human-enabled with post-collection analysis at US laboratory

Gaps in Current Technology

- Snapshot in time → lack of persistence, limited throughput
- Not suitable for difficult-to-access areas
- Requires constant human input

What We Need

- A small, low power, persistent, autonomous, remote chemical analysis capability
- Must have high sensitivity, wide dynamic range, and ability to identify ALL components of a complex mixture

We need to bring laboratory capabilities to the field

The Solution: MAEGLIN

Program Goal

Chemical identification in challenging environments with a small autonomous device

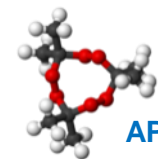
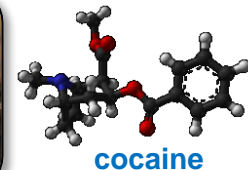
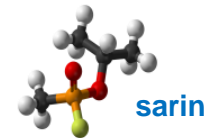
Compound Classes of Interest

- Chemical weapons
- Narcotics
- Nuclear fuel cycle materials
- Poisons
- Explosives



System Requirements

- 2-year unattended operation
- Daily sample analysis
- Autonomous & self-calibrating
- 1.5 liters & 7 kg (including power)
- 50-400 amu mass range
- High dynamic range separation
- Isotopic discrimination
- Gas, aerosol, and solid sample analysis
- Mass spectrometry NOT required





Potential Applications

User/Application	Details
Drug Enforcement	Monitoring effluent from suspected drug manufacturing sites for warrant issuance & evidence collection.
Domestic Counterterrorism	Monitoring effluent from suspected explosives, chemical agent, or bioagent manufacture or storage sites. Screening/early warning at large public gatherings.
Transportation Security	Testing cargo holds and package storage areas for illegal substances and explosives.
EPA/DOE	Monitoring of industrial and nuclear sites to enforce public safety and compliance standards; early warning system for inadvertent or intentional release.
Food and Pharmaceutical Security	Autonomous monitoring of food and drug production and storage to ensure safety and quality standards, lack of tampering.
Mining & Other Confined Spaces	Autonomous monitoring of safety conditions in mineshafts and other confined spaces.
Environmental Safety	Monitoring remote areas for illicit dumping of materials, unusual uses, early warning system for forest fires. Monitoring petroleum harvesting sites. Early warning system for volcanic eruptions.





MAEGLIN Technical Overview



How is it Done Now?

Past/Current Detection Programs	Description
Autonomous Rapid Facility Chemical Agent Monitor (ARFCAM)	Autonomous chemical detectors and networked systems to detect target compounds
Joint Chemical Agent Detector (JCAD)	Hand held detector that automatically detects, identifies and alarms to target chemicals
Lightweight Autonomous Chemical Identification System (LACIS)	Networked hand held chemical agent detectors for site assessment
Portable High-throughput Integrated Laboratory Identification System (PHILIS)	Mobile laboratory suite for high precision identification of chemicals for on-site analysis
Next Generation Chemical Detector (NGCD)	Detector alarms providing chemical event warning and improved vapor detection

Specific technologies used in autonomous detection include:

- Terahertz Spectroscopy
- IR/Raman
- GC-MS
- IMS
- Surface Acoustic Wave
- Photo- / Flame Ionization
- Polymer Detection Materials
- Electrochemical



Laboratory Systems for Complex ID

Common laboratory techniques for positive chemical ID:

- Nuclear magnetic resonance (mg sample sizes)
- Infrared Absorption Spectroscopy (μg sample sizes)
- Mass Spectrometry (ng-pg sample sizes)



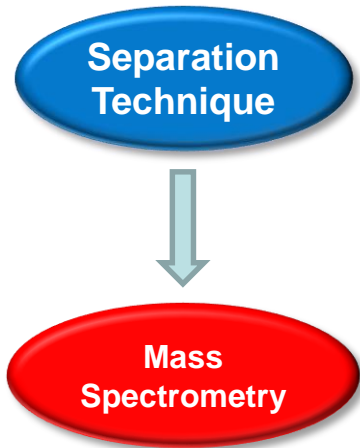
Capabilities common to all of these techniques:

- Uniquely identify a single chemical from a library of 100,000+ spectra
- Allow a trained spectroscopist to deduce a compound's structure from its spectrum
- Integrate a "front end" separation stage for complex samples, making interferences generally a non-issue



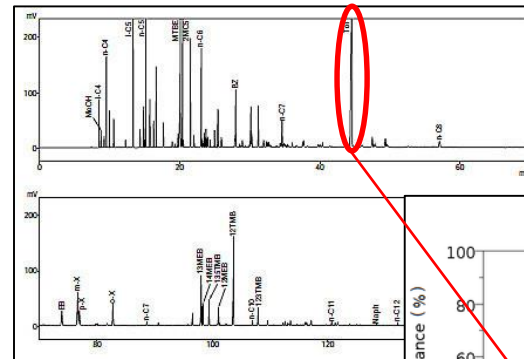
Hyphenated Mass Spectrometry

- Separation technique followed by mass-to-charge ratio analysis
- Common laboratory system for analysis of complex samples
- Increases dynamic range and enables ID of all components in a complex mixture with little to no sample preparation

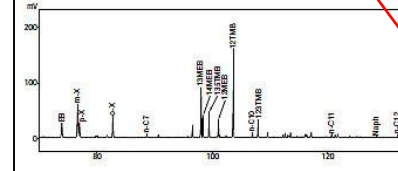


Complex mixture elutes as a series of temporally separated single-compound peaks

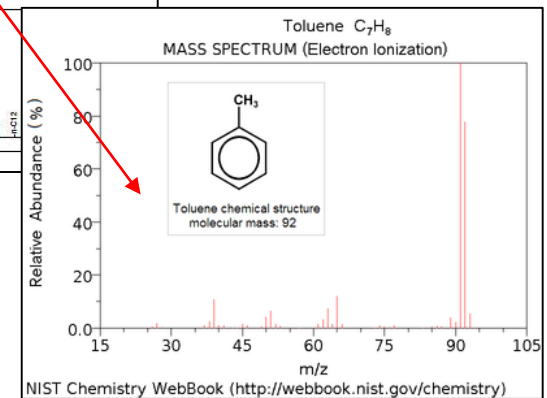
Molecular ions and ionic fragments detected as a function of their mass-to-charge ratio; specific chemical ID from fragmentation pattern



Chromatographic separation of gasoline fractions



Mass spectrum of toluene



High sensitivity / specificity, limited throughput and timeliness, high SWAP

Laboratory Separation Techniques

Technique	Description	Pros	Cons
Liquid Chromatography (LC, HPLC)	<p><i>HPLC System</i></p> <p>Liquid solvent pumped through solid stationary phase, interaction of mixture components w/ stationary phase determines transit time.</p>	<ul style="list-style-type: none"> • LC-MS is laboratory standard • Excellent separation 	<ul style="list-style-type: none"> • Large amount of consumables • Long analysis time
Gas Chromatography (GC)	<p>Interactions w/ stationary phase coated on capillary walls cause mixture components to slow by varying degrees during transit</p>	<ul style="list-style-type: none"> • GC-MS is laboratory standard • Excellent separation 	<ul style="list-style-type: none"> • Column compatibility • Column maintenance • Long analysis time • Humidity and dust may degrade columns
Ion Mobility Spectrometry (IMS)	<p>Separates ions by shape/size and charge</p>	<ul style="list-style-type: none"> • Fast analysis time • Separation on ion size 	<ul style="list-style-type: none"> • Potential problems in high humidity
Flow Cytometry	<p>Technology for analyzing the chemical characteristics of particles in a fluid as they pass through at least one laser beam, often using fluorescent labelling.</p>	<ul style="list-style-type: none"> • High through-put • Near real time analysis 	<ul style="list-style-type: none"> • Potential problems with volatile compounds • Large amount of consumables



What is Available for the Field?

Hand-held Mass Spectrometers

- 50–450 a.m.u.
- ~5 pounds; ~3 liters
- Ruggedized
- Low sensitivity and dynamic range
- Small battery & large power draw

Desktop / Portable Mass Spectrometers

- Limited ruggedness
- Heavy: 20–60 pounds
- Requires experienced user
- Large power draw

Other Technologies

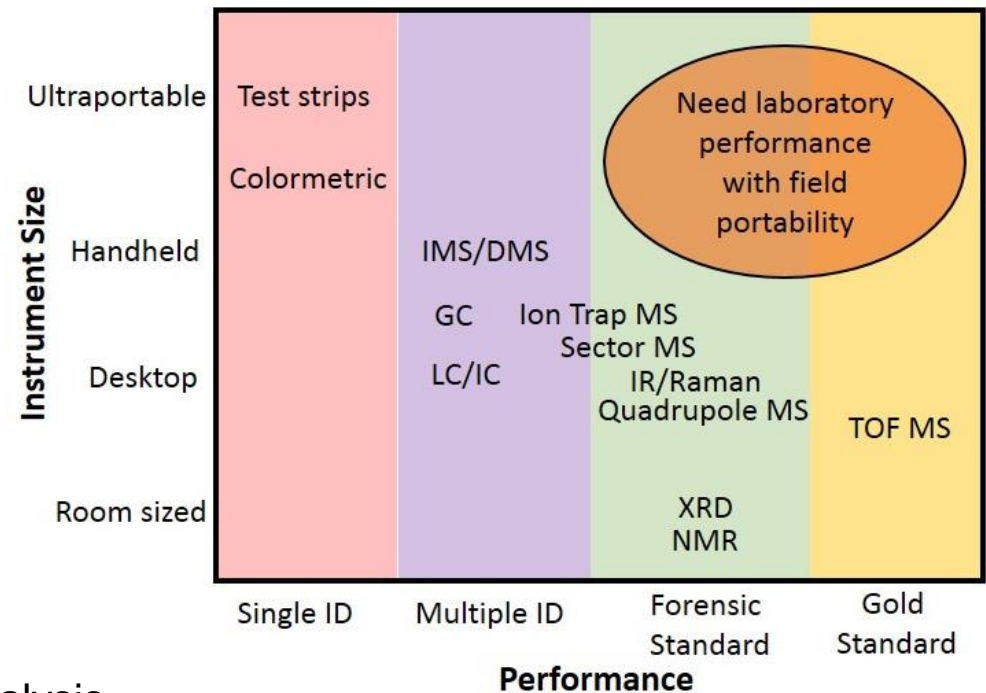
- Fluorescence, IMS, DMS, FTIR, Colorimetric, Raman
- Limited dynamic range & sample set
- Large power draw

Issues with Current Technologies

- Sensitivity
- Specificity; limited target set
- High power draw
- Insufficient resolution to ID a specific compound from a large library
- Strongly “tuned”; vulnerable to interferents

Current Limitations Summary

- **Non-mass spectrometry based chemical detection systems:** Cannot ID highly complex mixtures, handle extreme dynamic range, or discriminate isotopes
- **Field-portable mass spectrometry systems:** Achieved portability at the expense of sensitivity and selectivity; too power hungry for long-term emplacement.
- **Major power draws:**
 - Vacuum pumps
 - Mass analyzer
 - Ionization
- **Dealing with solids:**
 - Gas phase sample collection can be integrated and automated using pre-concentration on adsorbent media
 - Solid analysis requires “wet-lab” sample preparation or thermal analysis



Component Requirements & Key Enabling Technologies

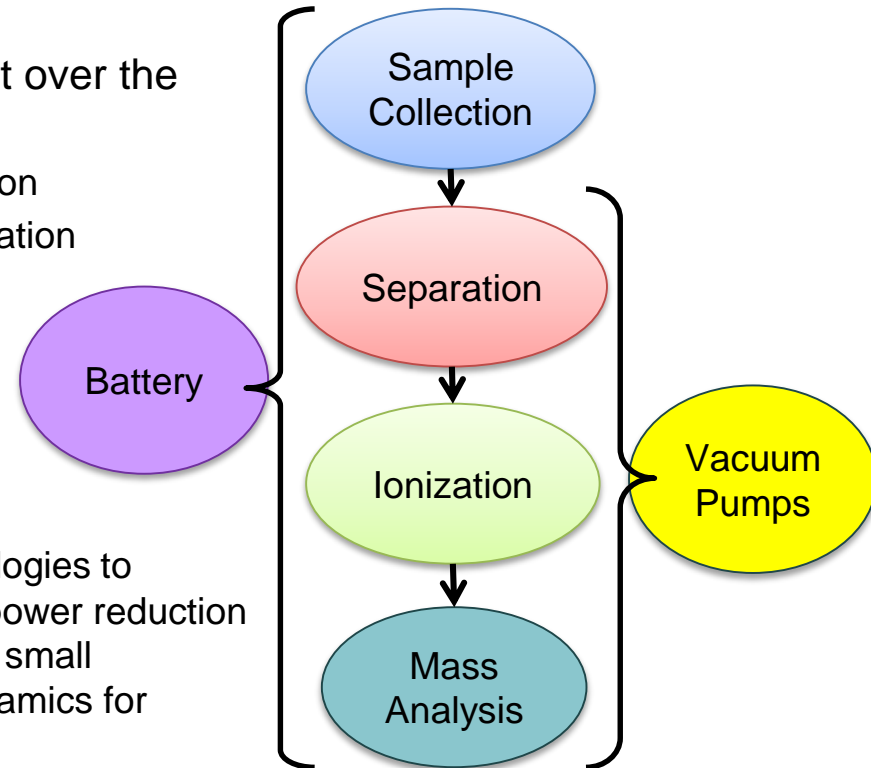
- **What makes MAEGLIN possible now?**

Achievements in relevant component development over the past 5-7 years:

- Gas phase adsorption: pre-concentration / volatilization
- Aerosol or solid phase collection/preparation/volatilization
- Separation
- Ionization
- Efficient mass analyzers
- Efficient and robust vacuum pump technology
- Batteries / power sources

- **Phase 1:** Development of advanced component technologies to provide robust system building blocks; proof of size and power reduction while meeting subcomponent sensitivity and selectivity in small breadboard system, consideration of interface & fluid dynamics for integration

- **Phase 2:** Prototype demonstration of integrated system with flexible, modular front end



Goal is lab performance in field portable device with ultra-low power draw

Component Requirements & Key Enabling Technologies

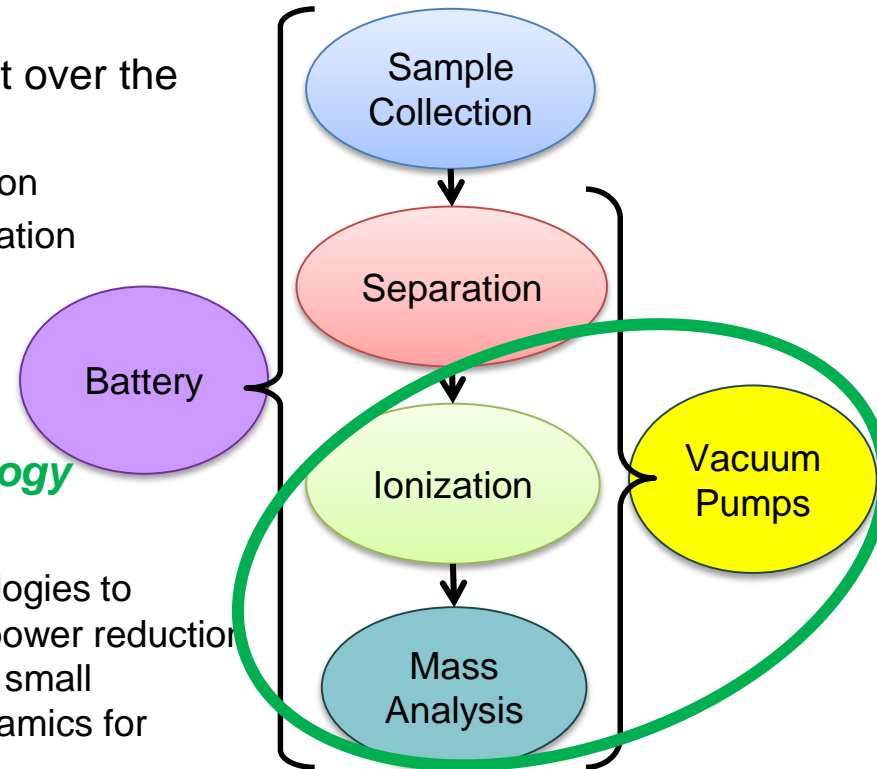
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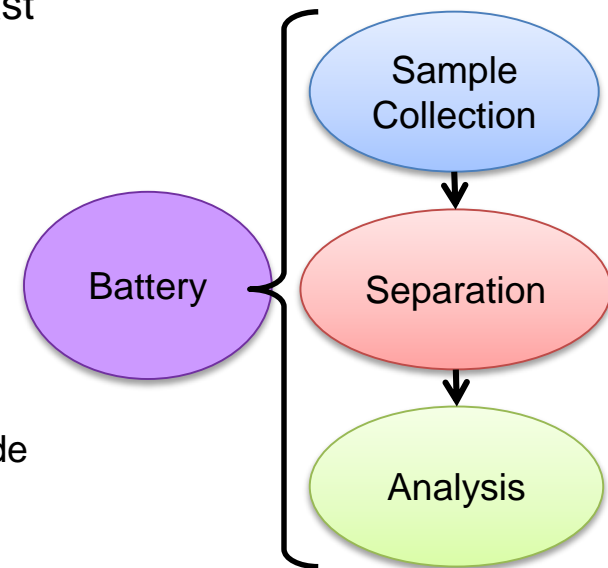
- **What makes MAEGLIN possible now?**

Achievements in relevant component development over the past 5-7 years:

- Gas phase adsorption: pre-concentration / volatilization
- Aerosol or solid phase collection/preparation/volatilization
- Separation
- **Alternative high specificity chemical ID method**
- Batteries / power sources

- **Phase 1:** Development of advanced component technologies to provide robust system building blocks; proof of size and power reduction while meeting subcomponent sensitivity and selectivity in small breadboard system, consideration of interface & fluid dynamics for integration

- **Phase 2:** Prototype demonstration of integrated system with flexible, modular front end



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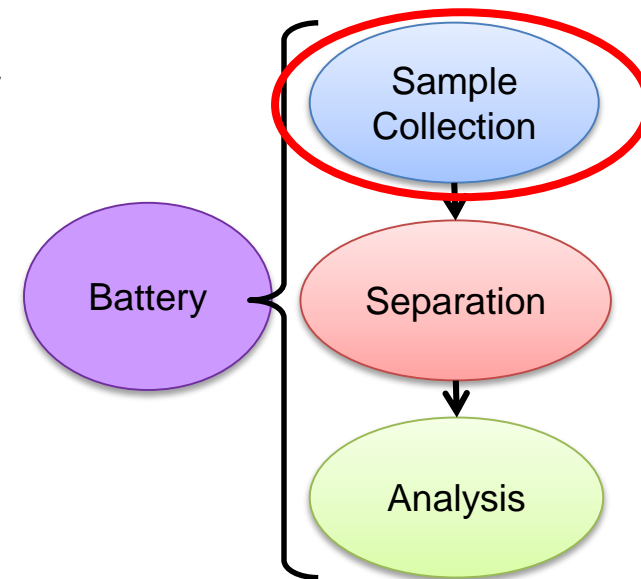
Sample Collection Thrust Area

Gas Phase collection requirements:

- Broad adsorptivity (volatiles, semivolatiles, polar, non-polar, ionic, etc.) – want to filter out major environmental gases
- Reusable (even best case will poison over time – consider remotely “changeable” cartridges for long term emplacement)
- Low power/essentially zero consumables required for release
- Release time and fluid dynamics appropriate for separation stage ingest

Aerosol / Solid / Liquid collection requirements:

- Modular front end adapter for handheld aerosol/solid/liquid sampling in the field
- Want maximum flexibility, limited consumables



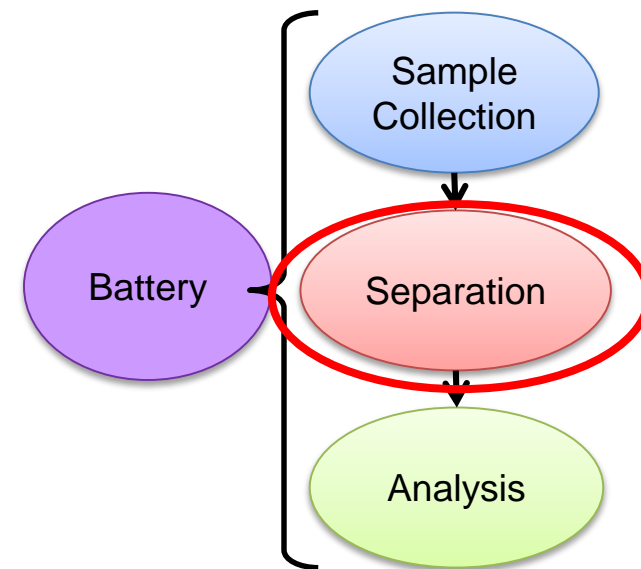
Separation Thrust Area

Separation requirements:

- Full or partial separation, must be sufficient to enable ID of all sample compounds with high dynamic range
- Need reduced power & size, reduced vacuum requirement, little or no consumables
- Small capillary devices increases susceptibility to clogging – need good pre-filter
- Separated compound chemical state and fluid dynamics appropriate for identification stage ingest

Representative technology approaches (not inclusive):

- μ -gas chromatograph (including “staged” versions)
- Miniature ion mobility spectrometer
- Miniature flow cytometer





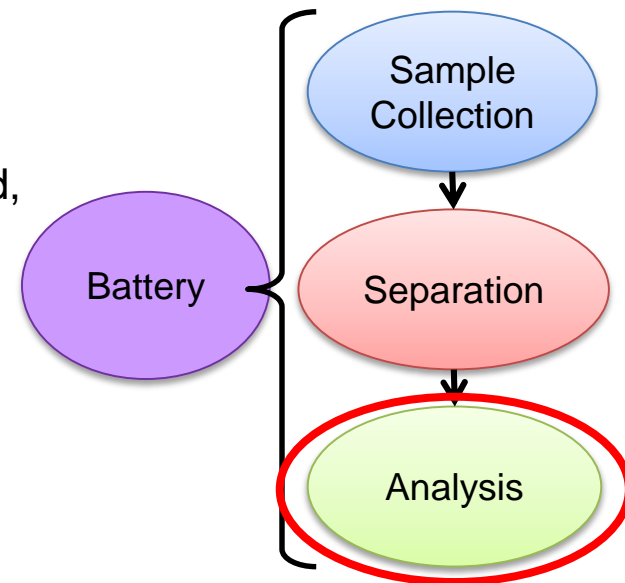
Analysis Thrust Area

- **Analysis requirements:**

- Absolute chemical ID (definitive signature) via adaptable on-board library
- Ability to identify existence of new compounds, record signature for offline analysis
- Technique amenable to self-calibration (internal standard, etc.)

- **Representative technology approaches (not inclusive):**

- Mass spectrometer – investigate reduced pumped area to enable higher pressure operation, passive components, array engineering
- Other ionization techniques
- Optical techniques

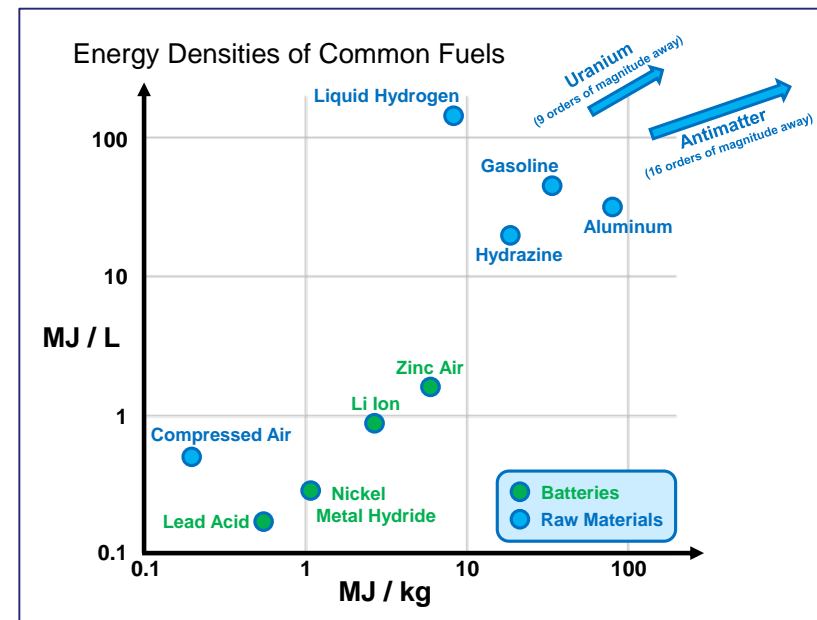




Ancillary Requirements: Vacuum and Power

- **Vacuum and Power are not direct investments for the MAEGLIN program, but overall system design should minimize the need for both**
- **Vacuum Pump Requirements:**
 - Small and power efficient
 - Resistant to vibration and shock
 - Flow rates compatible with atmospheric pressure inlets
- **Power Requirements:**
 - Primary goal is to minimize energy needs of all system components
 - High energy density batteries
 - Investigate potential for energy reuse/scavenging

DARPA Chip-scale Vacuum Micro Pumps (CSVMP) program developed microscale (as small as 0.5 cm³) vacuum pumps that operate at 10⁻⁶ Torr for integration with other MEMS and electronic components





MAEGLIN BAA Overview



Program Structure

- **Phase 1:** (18 Months)
 - Applied research in 3 thrust areas:

Collection	Separation	Identification
Low-power, reversible gas phase collection & pre-concentration. Modular adapter for solid / liquid phase collection & volatilization.	Non-destructive fractionation of chemical mixture with high dynamic range. Ability to “bleed off” all or part of selected fractions if desired. Low-power and minimal (preferably no) consumables.	High accuracy identification of pure compounds and low-count mixtures. Large and adaptable library. Low-power and minimal (preferably no) consumables.

- **Phase 2:** (18 Months)
 - Integrated prototype demonstration
 - Show low-power collection, separation, and identification of chemical sample targets.



BAA Highlights

- Separate BAAs for Phases 1 and 2
- Offeror team must address all of program requirements within a thrust area; no partial proposals, such as development of specific component technology, will be accepted
- May bid to 1, 2, 3 thrust areas – separate proposals for each
- The Government anticipates that proposals submitted under this BAA will be unclassified
- Multiple awards are expected
- Foreign participants and/or individuals may participate to the extent that such participants comply with any necessary Non-Disclosure Agreements, Security Regulations, Export Control Laws and other governing statutes applicable under the circumstances



Metrics for Phase 1 Thrust Areas

Thrust Area	Metric / Performance
All	<ul style="list-style-type: none">• Library: 50 targets, 100 background compounds, 5 true unknowns; compound mass range 50-400 amu; polar, non-polar, volatile, semi-volatile compounds; library will include both physical (retention time) and functional (similar spectra) challenges• Size: For each component, traceable to a 0.5 L package (or 1.5 L total). Demonstration can be larger breadboard, but must include drawing/model showing clear path to Phase 2 packaged size• Power: Threshold <5 W per component; goal <1 W per component
Collection	<p><u>Gas phase (required)</u></p> <ul style="list-style-type: none">• Input: Ambient air• Output: Neutral gas phase bolus• Concentration range: Minimum 50 ppt (pg/cm²), maximum 500 ppm (µg/cm²)• Sample time: Minimum 30 minutes, maximum 24 hours• Release time: 0.25 seconds• Single cartridge reuse: Threshold 75X, goal 750X• Other: No chemical reactions or degradation during storage or release, minimal consumables (none preferred) <p><u>Aerosol, liquid, and/or solid phase</u></p> <ul style="list-style-type: none">• Form factor: Modular, removable adaptor on gas phase collector; additional 0.25 L volume allowed per adaptor; minimal consumables (none preferred)



Metrics for Phase 1 Thrust Areas *cont.*

Thrust Area	Metric / Performance
Separation	<ul style="list-style-type: none">• Input: Neutral gas phase bolus• Output: Neutral species or molecular ions• Throughput: greater than 50%• Separation: Threshold - fractions containing no more than three individual compounds, goal - fully separated fractions• 10,000X or greater, with bleed off capability to reduce high concentration species
Identification	<ul style="list-style-type: none">• Input: Neutral species or molecular ions; both pure compounds and low count mixtures• Output: Automated compound ID capability (non-real time)• Detectable Concentration: Minimum: 10 ppb (ng/cm²), maximum: 10 ppm (µg/cm²)• Resolution:<ul style="list-style-type: none">- Mass Spectrometry based systems: 0.3 amu, isotopic analysis capability desirable- Non-MS based systems: Discrimination of all library spectra with <0.01% probability of misidentification



Anticipated Metrics for Phase 2 Integrated Prototype

Metric	Performance
Mass Range	<ul style="list-style-type: none">50-400 amu
Resolution	<ul style="list-style-type: none">Mass spectrometry based systems: 0.1 amu, isotopic analysis capability requiredNon-mass spectrometry based systems: Discrimination of all library spectra with <0.01% probability of misidentification
Specificity / Interference	<ul style="list-style-type: none">100 targets with background of 400 materialsDesign library to include both physical (retention time) and functional (similar spectra) interference challenges
Targets (including standardized sets)	Semivolatiles (EPA method 625) Organophosphate pesticides (EPA method 8141B) Volatile organic compounds (EPA method 8260B) Diesel and gasoline exhaust Chemical warfare agents, toxic industrial chemicals, and their precursors Explosives/energetics target set Narcotics target set
Probability of Detection (P_d)	<ul style="list-style-type: none">>95% at Minimum Detectable Concentration
Probability of False Alarm (P_{fa})	<ul style="list-style-type: none"><0.01% Probability of Misidentifying Target/Background



Anticipated Metrics for Phase 2 Integrated Prototype, *cont.*

Metric	Performance
Size, Weight, Power	<ul style="list-style-type: none">• <1.5 L, with no dimension >30cm (including power)• <7 kg• 2 years on battery/fuel cell or energy scavenging
Communications	<ul style="list-style-type: none">• Internal instrument control for calibration, pulsed sampling• Storage capacity for 6,000 sampling events• Raw data accessibility and portability for off-system analysis• Efficient data export format
Environmental	<ul style="list-style-type: none">• Audio Noise: <20 dBA• EMF: <0.1 milliGauss, <1V/m outside package• Heat Dissipation: <1W
System Operability	<ul style="list-style-type: none">• Automated internal calibrant/calibration procedure• Automated clear-down procedure following large hit
Atmospheric Inhibition	<ul style="list-style-type: none">• Minimal/no impact (<1% error) on P_d and P_{fa} caused by humidity, temperature, dust, and altitude.
Data storage	<ul style="list-style-type: none">• System must be able to store complete compound libraries• System must be able to store and compare to data collected from the last 14 runs



Milestones and Waypoints

- **Milestones** are Government-defined progress metrics that must be met by the end of each phase
- **Waypoints** are offeror-defined, task-driven intermediate steps towards a milestone
 - Depending on an offeror's specific approach, progress towards a milestone is not expected to be linear in all areas
 - Waypoints are how the offeror clearly explains to the Government the quantitative and timely progress that must be made for their overall concept to meet the end-of-phase Milestones – performance against these waypoints is reviewed throughout program
- **Technical reviews** held at months **3, 5, 8, 11, and 14** will quantify progress against the waypoints & assess whether course corrections are needed for success



GFI/GFE – Phase 1

- **At Contract Award:**
 - List of target and background chemicals
- **Months 11 and 16:**
 - Test samples with full metadata - appropriately formulated for each thrust area



T&E/Deliverables – Phase 1

- **Months 3, 5, 8, 11 & 14** – Progress review against offeror-defined waypoints (emphasis on months 5 and 11)
- **Month 15** – Report on traceability of component design to Phase 2 goals, inlet/outlet characteristics and requirements
- **Month 17** – Test system against Government provided samples
- **Month 17** – System available for independent Government testing
- **Month 18** – Final report & hardware/software deliverable.



Notional/Target Schedule

