Advanced Water-Splitting Technology Pathways Benchmarking & Protocols Workshop

Breakout Session Summaries
Thermo-Chemical Hydrogen (TCH)

June 11 – 12, 2024

TCH Breakout Sessions

Session ID	Topic	Lead	Note Taker
S1	TCH Metrics	Michael Sanders (Mines)	Kent Warren (U Colorado)
S2	Test Protocols and Publications	Sean Bishop (Sandia)	Kent Warren (U Colorado)
S3	Value Proposition and Roadmap	Sean Bishop (Sandia)	Kent Warren (U Colorado)
S5	Thermo-electro-chemistry	Jim Miller (ASU)	Sean Bishop (SNL)

Session Summary

Session ID: STCH-1

Title: Metrics

Summary of discussion

- Power density (MW/kg, MW/m³) is the best metric for comparing technologies.
- Choose different conditions for final hydrogen output; split metrics by pressure and hydrogen purity.
- Capture capital equipment and active material supply chain vulnerability and volatility as metrics.
- Include balance of plant considerations in CAPEX and efficiency calculations.
- Use capacity factor to differentiate continuous and diurnal production; other metrics may be better.
- Technology metrics should not focus on CO_2 produced per hydrogen, as these values are installation-specific.

Consensus and/or dissenting opinions

- Consensus: Agreement was found on the basic list of metrics.
- Dissenting Opinions: There was some disagreement on how to normalize for different approaches, especially when comparing different input energy sources (grid vs. solar vs. "waste" heat).

Key takeaways

- While there is agreement on the need for metrics to compare hydrogen production approaches, it is unlikely that a single metric can fully describe the benefits and trade-offs across all relevant categories.
- A group of 4-5 different metrics with a few sub-metrics for some may be sufficient.
- The list given above is a reasonable starting point, but further development needs to include comparisons to other technology tracks.

Action Items

- No action items assigned

Session Attendee List

Session ID: STCH-1

Title: Metrics

Name	Affiliation
Aaron Overacker	SNL
Alberto de la Calle (online)	CSIC
Alicia Bayon (online)	CSIC
Ari Clauser	SNL
Ellen Stechel	ASU
Eric Coker	SNL
James Miller	ASU
Katherine Rinaldi	DOE
Keith King	SNL
Kent Warren (session scribe)	CU-Boulder
Matthew Witman	SNL
Michael Sanders (session lead)	Colorado School of Mines
Nicholas Strange	SLAC
Sean Bishop	SNL
Shang Zhai	OSU
Tyra Douglas	SNL

Session Summary

Session ID: STCH-2

Title: Test Protocols and Publications

Summary of discussion

- Develop and publish protocols in a new Frontiers special issue.
- Consider a summary of TCH analytical tools as a protocol.
- Develop round-robin testing, requiring protocols and exemplar materials for validation.

Consensus and/or dissenting opinions

Consensus:

- Balance scientific merit with applied research in the publication format; scientific reasoning of protocol background should address this balance
- Consider developing a flow reactor protocol to include non-flow reactor type measurements for round-robin testing (only two SFRs for TCH exist).

Dissenting Opinions:

- Develop a computational-based protocol described in terms an experimentalist can understand, such as which oxygen vacancy formation energy to use when multiple oxygen sites are reported by DFT.

Key takeaways

- Exemplar materials identified for round-robin testing: CeO_2 and $La_{0.8}Sr_{0.2}MnO_{3-\delta}$ (LSM20).
- Previously published but not widely accessible protocols (e.g., in books) can be referenced in protocol validation via round-robin tests in new publications.
- Durability protocol is challenging; consider three stages of durability: preliminary evaluation via inert+oxygen cycling, followed by more complex evaluations involving controlled steam or CO_2.

Action Items

- Flow reactor protocol (Keith, Tony, Kent)
- HTXRD protocol (Tyra, Sean, Eric)
- Machine learning cross validation protocol (Matt)
- Initiate round-robin testing of exemplar materials (e.g., use TGA TCH protocol)

Session Attendee List

Session ID: STCH-2

Title: Value Proposition and Roadmap

Name	Affiliation
Aaron Overacker	SNL
Alberto de la Calle (online)	CSIC
Alicia Bayon (online)	CSIC
Ari Clauser	SNL
Ellen Stechel	ASU
Eric Coker	SNL
James Miller	ASU
Katherine Rinaldi	DOE
Keith King	SNL
Kent Warren (session scribe)	CU
Matthew Witman	SNL
Michael Sanders	CSM
Nicholas Strange	SLAC
Rob Wexler (online)	WUSTL
Sean Bishop (session lead)	SNL
Shang Zhai	OSU
Tyra Douglas	SNL

Session Summary

Session ID: STCH-3

Title: Value Proposition and Roadmap

Summary of discussion

- Focused on high-level metrics across technologies rather than TCH-specific metrics (covered in previous meetings).
- Examined the value proposition for TCH and why it should continue to receive DOE attention.
- Discussed the roadmap for TCH to evaluate high-level metrics.

Consensus and/or dissenting opinions

Consensus:

- Removing the constraint of solar on TCH is a positive. For example, TCH can utilize process heat when integrated with existing industrial processes.
- Increased industrial engagement is needed to identify their needs and paths for TCH integration.

Dissenting Opinions:

- It is not clear what a scalable reactor design should be or how many variants should be considered in Technoeconomic analyses

Key Take-Aways

- Industry familiarity with thermo-chemical processes is a key selling point for TCH commercialization.
- TCH being volumetric has better scalability than 2D modular technologies.
- Reactor design and testing have been limited and need to be included in a roadmap.
- Hydrogen production metrics need to consider H_2 production/plant mass, supply chain vulnerabilities, and the type of H_2 produced (e.g., purity, pressure).
- Industry often seems unaware of TCH as an option for H_2 production.

Action Items

- Develop multiple reactor designs for on-sun testing via consortium seedling-lab interactions (Tony+Sean leads)
- Evaluate TEA of different TCH approaches via consortium seedling-lab interactions (Zhiwen Ma-NREL lead)
- Continue to engage with industry (Ellen and Kent)

Session Attendee List

Session ID: STCH-3

Title: Value Proposition and Roadmap

Name	Affiliation
Aaron Overacker	SNL
Alberto de la Calle (online)	CSIC
Alicia Bayon (online)	CSIC
Ari Clauser	SNL
Ellen Stechel	ASU
Eric Coker	SNL
Huyen Dinh	NREL
James Miller	ASU
Karl Gross	SNL
Katherine Rinaldi	DOE
Keith King	SNL
Kent Warren (session scribe)	CU
Matthew Witman	SNL
Michael Sanders	CSM
Nicholas Strange	SLAC
Rob Wexler (online)	WASHU
Sean Bishop (session lead)	SNL
Shang Zhai	OSU
Tyra Douglas	SNL

Session Summary

Session ID: STCH 5

Title: Thermo-Electro-Chemical

Summary of discussion

- Hybrid thermochemical and electric-driven redox
  - Shift reaction equilibrium with direct electrical input
  - May offer the best of each while overcoming barriers
  - Potential pitfalls: complexity, reduced efficiency
- Limited examples of work in this area
- Many different options for implementation
  - Electrically boost reduction
  - Electrically boost oxidation
  - Indirectly shift equilibrium by electrochemical pumping or separation
  - Molten salt/metal, membranes, layered structures
- - TNSTAAFL – theoretical energy required is unchanged

Consensus/Dissenting Opinions

Consensus:

- Dividing line between TCH and electrolysis needs clarification.
- At first glance, known materials for different functions (redox vs. ion transport, etc.) have different optimum temperatures.

Dissenting Opinions:

- What is the best approach (intuitively may be separation) – is it too early to define that?
- Is this detracting from the work we are already making good progress with?
- Can we integrate with chemical synthesis as a driving force?

Key Take-Aways

- Worth pursuing/refining idea
- Consistent with the name change from STCH to TCH

Action Items

- Apply knowledge of thermodynamics and economics to evaluate advantages and disadvantages.
- Identify potential areas for development and needs.
- Consider other options not discussed today.

Session Attendee List

Session ID: STCH 5

Title: Thermal/Chemical STCH

Name	Affiliation
Aaron Overacker	SNL
Ari Clauser	SNL
Ellen Stechel	ASU
Eric Coker	SNL
Jim Miller (session lead)	ASU
Kat Rinaldi	DOE
Keith King	SNL
Matt Witman	SNL
Michael Sanders	CSM
Nick Strange	SLAC
Sean Bishop (session scribe)	SNL
Shang Zhai	OSU
Tyra Douglas	SNL

Session Summary

Session ID: C4-B
Title: Setting Common Metrics for LTE, HTE, PEC, STCH

Summary of discussion

- Current metrics are specific to technologies and not relevant across different technologies.
- Goal: Establish a common set of metrics (4-5) applicable to all pathways.
- Motivation: Aid DOE and customers in understanding pros and cons, drive towards a dollar/kg metric, and demonstrate the value of diverse pathways.
- Specific metrics discussed:
  - H2 metrics: Low and high pressure, low and high purity (e.g., 99.999% vs. 99.6% purity, 30 bar vs. atmospheric pressure).
  - Energy input comparison: kWh/kg with consideration for technology differences.
  - Power density: Mass footprint and volume considerations, conversion factors for reporting.

Consensus/Dissenting Opinions

Consensus:

- Common H_2 metrics for purity and pressure levels.
- Bar chart for showing solar, electricity, and heat inputs
- Power density to be reported with clear conversion factors (ΔG^0, HHV, LHV).

Dissenting Opinions:

- kWh input comparison may unfairly disadvantage solar technologies when compared to electricity-based technologies.
- Debate on how to fairly compare exergy between solar and electricity-based technologies.

Key Take-Aways

- Establishing common metrics is crucial for cross-technology evaluation.
- Agreed upon metrics for hydrogen purity and pressure levels.
- Use kWh/kg for energy input with clear understanding of its limitations.
- Importance of reporting power density with explicit conversion factors.
- Need for a visual representation (e.g., bar chart) for energy input comparisons.

Action Items

- Finalize the set of common metrics (4-5) for all pathways.
- Develop a methodology for comparing kWh input across different technologies and inputs
- Create guidelines for reporting power density with specified conversion factors.
- Design and circulate a bar chart template for visualizing energy input comparisons.
- Address unresolved issues around exergy comparisons in future discussions.

Session Attendee List

Session ID: STCH 5

Title: Thermal/Chemical STCH

Name	Affiliation
Aadarsh	CSM
Aaron Overacker	SNL
Ari Klauser	SNL
Elias Pomeroy	DOE
Eric Coker	SNL
Flavio da Cruz	SoCalGas
Huyen Dinh	NREL
Jeremy Hartvigsen	INL
Jim Miller	ASU
Kai Outlaw-Spruell	UH
Kat Rinaldi	DOE
Keith King	SNL
Kiram Adepalli	Nexceris
Long Le	PNNL

Session Attendee List

Session ID: STCH 5

Title: Thermal/Chemical STCH

Name	Affiliation
Matt Whitman	SNL
Michael Sanders	CSM
Nick Strange (session secondary scribe)	SLAC
Sarafina Fortiner	NEL
Sarah Shulda (session primary scribe)	NREL
Sean Bishop	SNL
Tadashi Ogitsu	LLNL
Todd Deutsch	NREL
Tyra Douglas	SNL