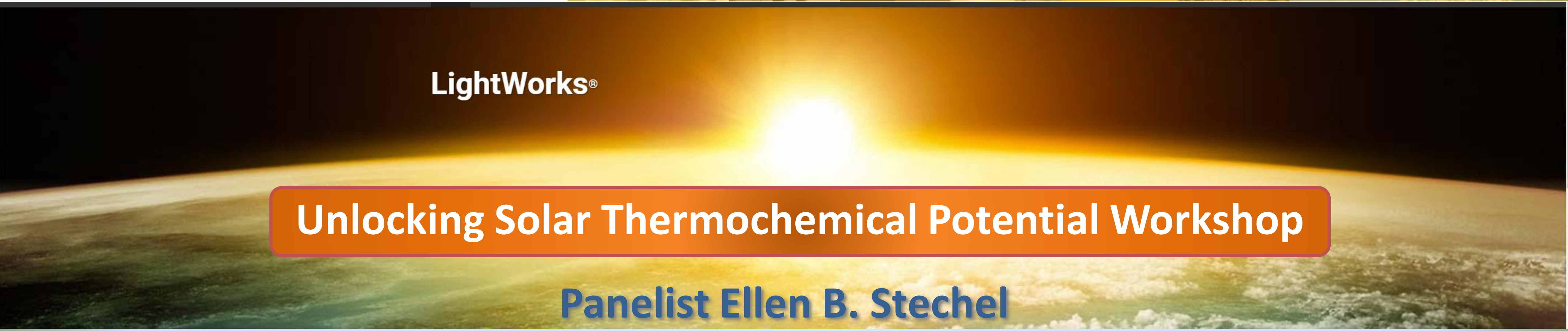


Unlocking Solar Thermochemical Potential Workshop

Panelist Ellen B. Stechel

ASU LightWorks®, Arizona State University, Tempe AZ, USA

COLLABORATORS

Arizona State University: Shuguang Deng, Ivan Ermanoski, James E. Miller, Ryan Milcarek, Chris Muhich
Georgia Institute of Technology: Peter Loutzenhiser
National Renewable Energy Laboratory: David Ginley, Karen Heinselman, Bob Bell, Phil Parilla, Dan Plattenberger, Sarah Shulda
Oregon State University: Brian Fronk
Princeton University: Emily Carter (now UCLA), Sai Gautam (now IISc), Rob Wexler
Sandia National Laboratories: Kevin Albrecht, Andrea Ambrosini, Evan Bush, Eric Coker, Matt Kury, Tony McDaniel
Siemens Corporation: Ioannis Akrotirianakis, Arindam Dasgupta, Ayse Parlak
Southwest Research Institute: Stefan Cich, Josh Neveu

SOLAR THERMOCHEMISTRY CONTEXT

- **Chemistry**: Making and breaking bonds
- **Thermochemistry** combines the concepts of thermodynamics with the idea of energy in the form of chemical bonds.
- **Thermochemistry** is a branch of **thermodynamics** that is the study of heat generated (exotherm) or consumed (endotherm) in a **chemical reaction**.
- **Solar**: Source of heat particularly to promote the endothermic reactions

Heat can also accelerate reactions even if exothermic

High temperature can be sustainable when enabled by solar fuels or concentrated solar

- **Deep Decarbonization:** Applications to a large range of carbon-intensive sectors
- **Dispatchability:** Enable deeper penetration of renewables with less curtailment

SOME (MANY) APPLICATIONS OF SOLAR THERMOCHEMISTRY

Thermochemical Storage	Solar Fuels	Commodities
Redox Cycles Hydration/ De-Hydration Carboxylation/ De-Carboxylation	Redox Cycles: Water and Carbon Dioxide Splitting Reforming/ Gasification Chemical Looping with CH_4	Redox Cycles: Air Separation Calcination Metal Ore Reduction
Heat for power cycles (air Brayton or sCO_2 Brayton) or other high temperature industrial processes	*Hydrogen (H_2), Carbon Monoxide (CO), Syngas (H_2/CO/CO_2 mix) Methanol (CH_3OH), DME (O=$(CH_3)_2$), Diesel, Jet Fuel, NH_3, Co-produce H_2 / e^-*	*Metals (Fe, Al, Zn, Cu, Li) Steel, Cement, lime, Pure Nitrogen (N_2), Pure Oxygen (O_2), Ammonia (NH_3)*

SOME THERMOCHEMICAL REACTIONS OF INTEREST

Redox: Oxygen Shuttle

$$\frac{1}{\delta}\mathrm{MO}_x \rightarrow \frac{1}{\delta}\mathrm{MO}_{x-\delta} + \frac{1}{2}O_2$$

$$CH_4 + \frac{1}{\delta}\mathrm{MO}_x \rightarrow \frac{1}{\delta}\mathrm{MO}_{x-\delta} + CO + 2H_2$$

$$H_2 + \frac{1}{\delta}\mathrm{MO}_x \rightarrow \frac{1}{\delta}\mathrm{MO}_{x-\delta} + H_2O$$

$$\frac{1}{\delta}\mathrm{MO}_{x-\delta} + H_2O \rightarrow \frac{1}{\delta}\mathrm{MO}_x + H_2$$

$$\frac{1}{\delta}\mathrm{MO}_{x-\delta} + CO_2 \rightarrow \frac{1}{\delta}\mathrm{MO}_x + \mathrm{CO}$$

$$\frac{1}{\delta}\mathrm{MO}_{x-\delta} + Air \rightarrow \frac{1}{\delta}\mathrm{MO}_x + N_2$$

Thermochemical Energy Storage

$$\frac{1}{\delta}\mathrm{MO}_x \rightleftarrows \frac{1}{\delta}\mathrm{MO}_{x-\delta} + \frac{1}{2}O_2$$

$$CaCO_3 \rightleftarrows CaO + CO_2$$

$$Ca(OH)_2 \rightleftarrows CaO + H_2O$$

Thermochemical Ammonia

$$\frac{1}{\gamma}\mathrm{MN}_x + \frac{3}{2}H_2 \rightarrow \frac{1}{\gamma}\mathrm{MN}_{x-\gamma} + NH_3$$

$$\frac{1}{\gamma}\mathrm{MN}_{x-\gamma} + \frac{1}{2}N_2 \rightarrow \frac{1}{\gamma}\mathrm{MN}_x$$

Gasification

$$C_xH_{2y}O_z + (x-z)H_2O \rightarrow (y+x-z)H_2 + xCO$$

Reforming

$$CH_4 + H_2O \rightarrow \mathrm{CO} + 3H_2$$

$$CH_4 + CO_2 \rightarrow 2\mathrm{CO} + 2H_2$$

Each application presents different challenges at the system level but many commonalities too

Important to co-optimize materials, reactors, desired operating range, and the systems

KEY RISKS OFTEN OVERLOOKED EARLY IN THE DEVELOPMENT PROCESS

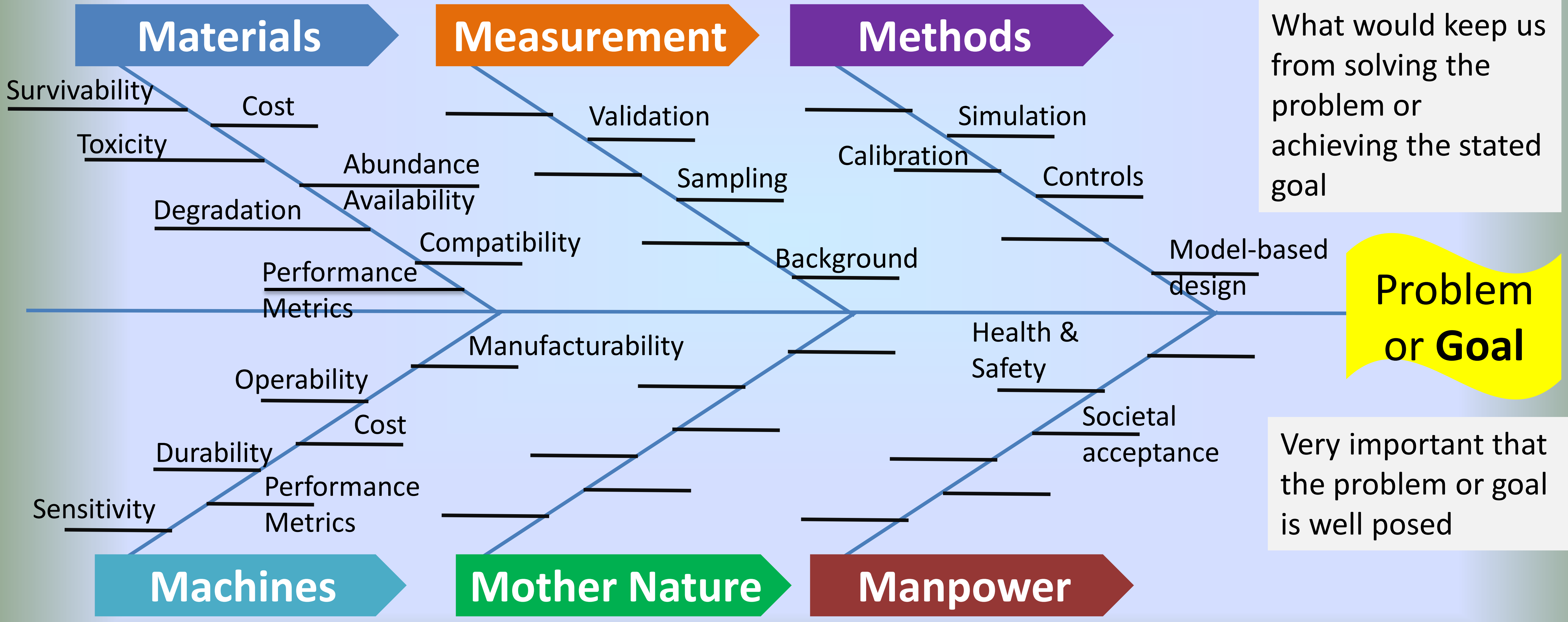
Having a good technical risk assessment and review formalism

- Identifying all the possible failure modes – what would keep the material, the functional components, interfaces, or the system from working as intended?

Potential Failure mode	Potential Effect(s) of Failure	Severity (1-10)	Potential Mechanism(Causes) of Failure Mode	Occurrence (1-10)	Current Design Features/ Controls	Detection (1-10)	Risk Priority Number (RPN)	Recommended Actions

- The FMEA (Failure Mode Effects & Analysis) is a collaborative exercise and works best with a diverse team
- Can be effective at identifying and mitigating or eliminating risks
- Applies broadly, e.g., to design of functional materials, components, interfaces, and the full system
- Early on – sufficient to drive the RPN = Severity × Occurrence × Detectability < 100

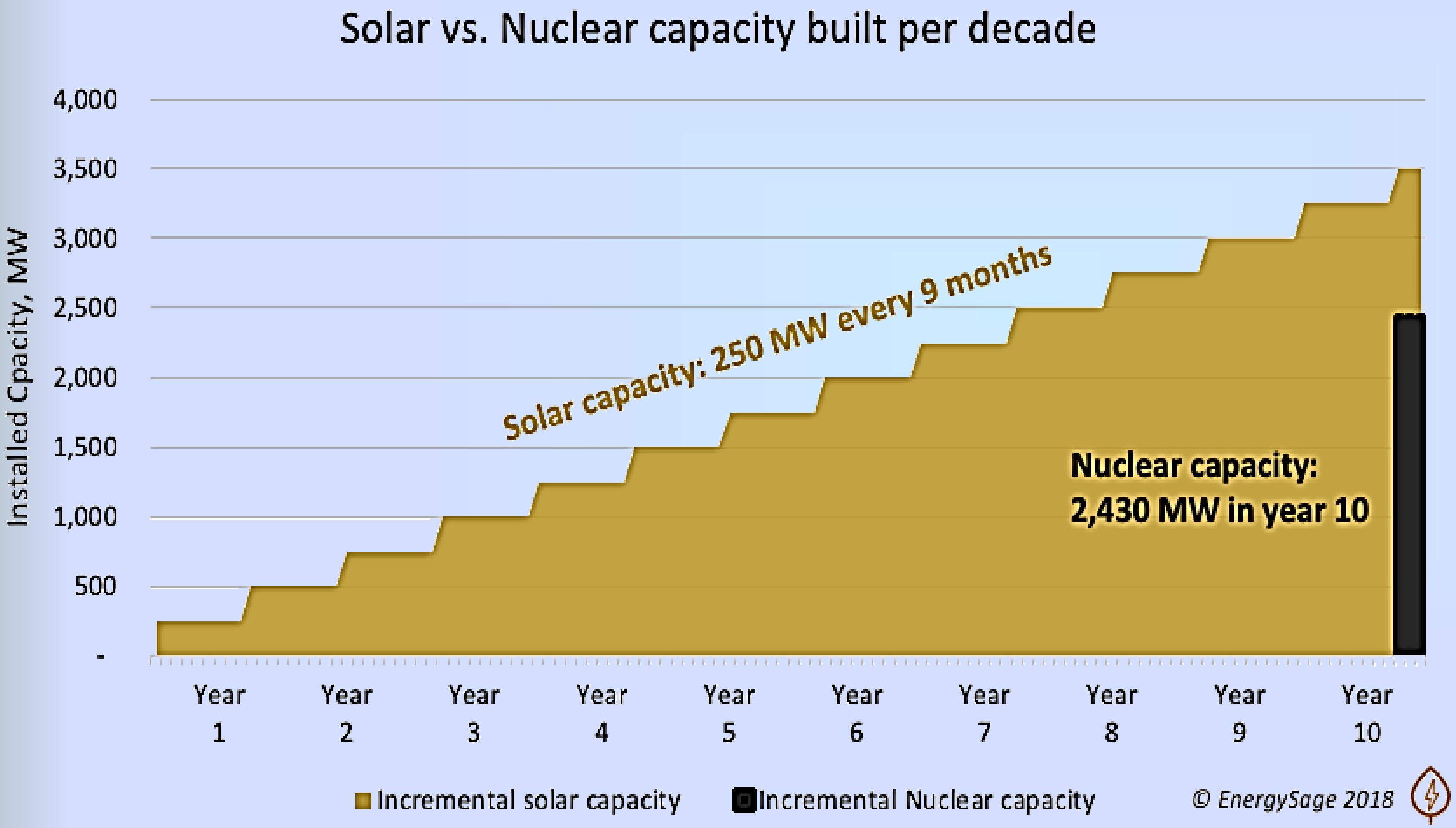
FISHBONE DIAGRAM CAN AID IN ASSESSING RISKS



What would keep us from solving the problem or achieving the stated goal

Very important that the problem or goal is well posed

VERY IMPORTANT RISK IS GETTING THE SCALE RIGHT



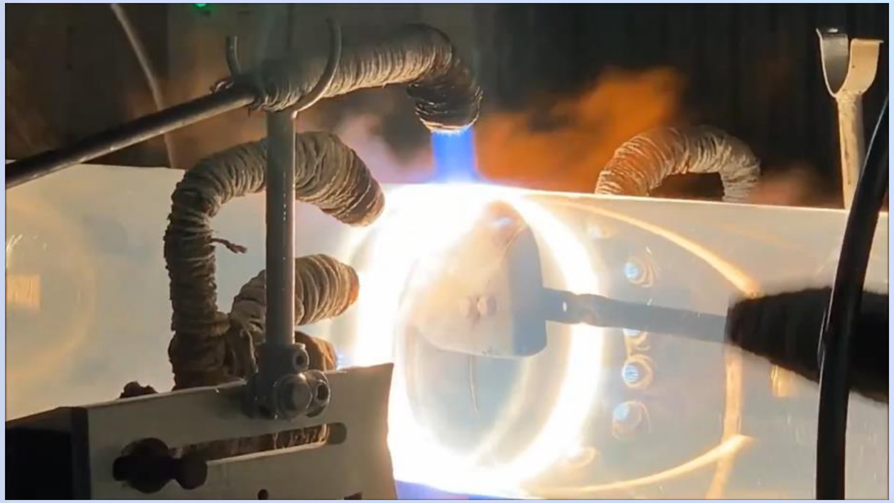
- Flexibility, Adaptability
- Faster Learning
- Less Investor Risk
- Start generating revenue more quickly
- Matching scale with downstream processing, e.g., syngas → jet fuel

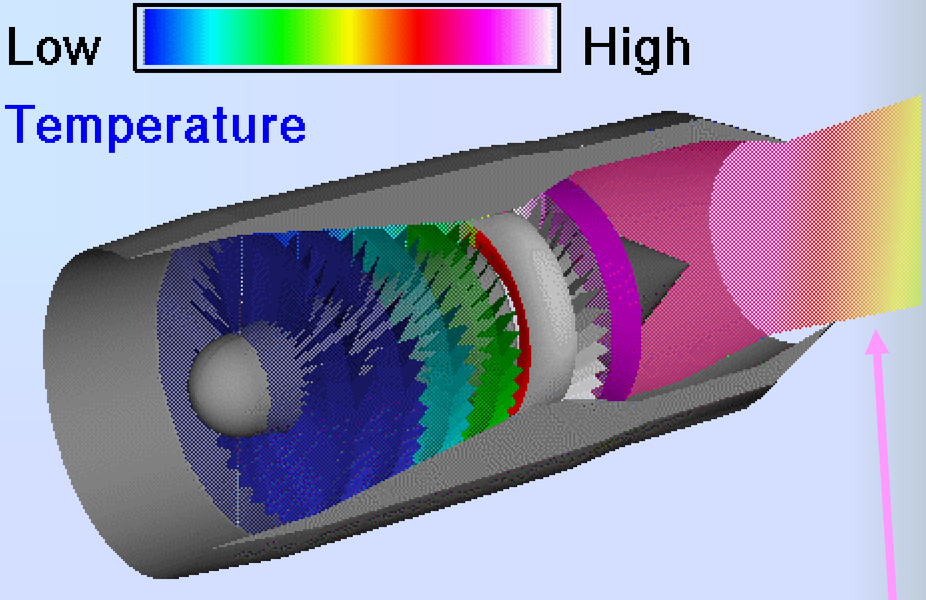
RISK OF NOT OPTIMIZING FOR THE THERMODYNAMICS BECAUSE OF HIGH TEMPERATURE

Challenging but not necessarily a show-stopper: Know the difference between an engineering challenge that might have analogs in other applications and show-stoppers

High Temperature Industrial Processes

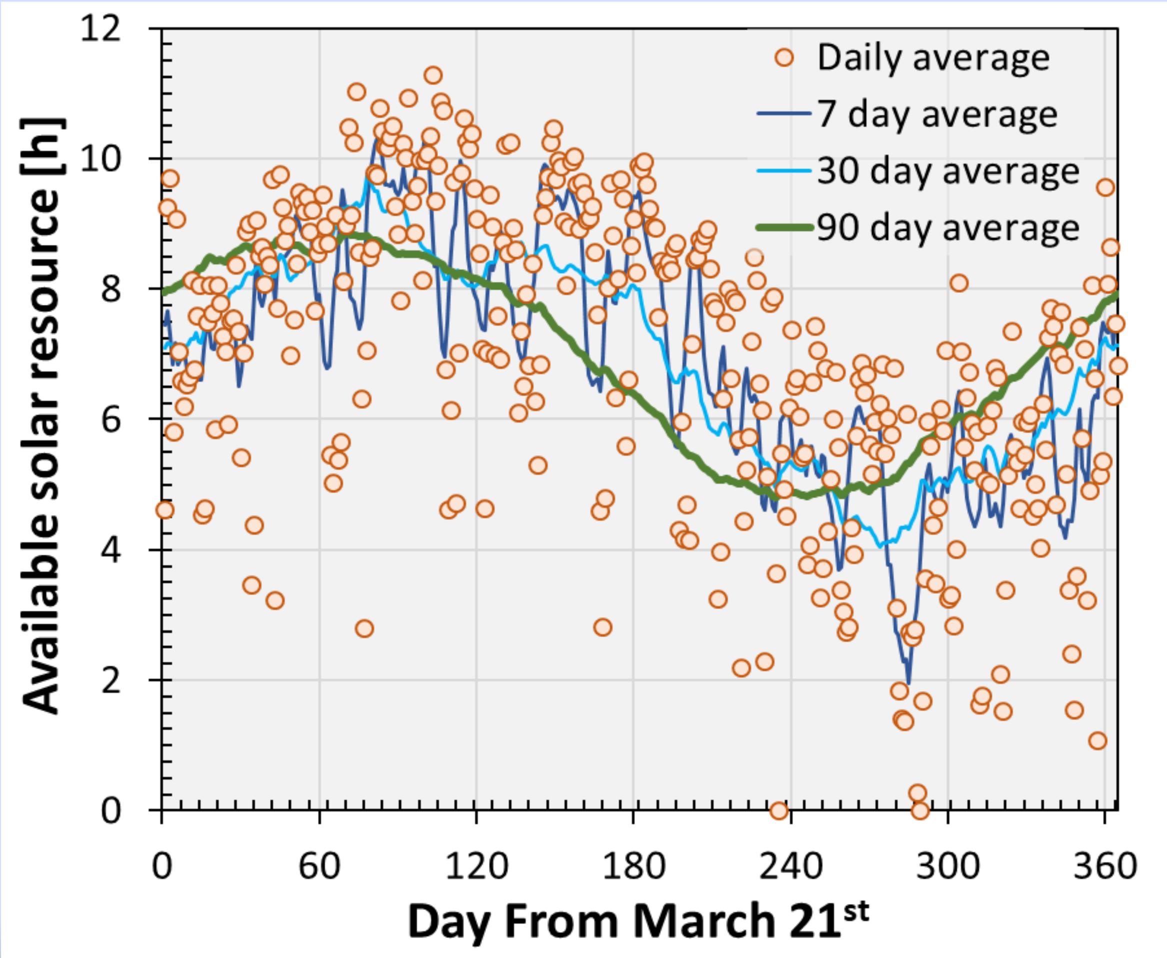
Fusing quartz under H_2/O_2 flame: T~1700°C





Jet turbine inlet temperature: ~1600°C

REGIONS WITH AN EXCELLENT SOLAR RESOURCE STILL MUST COPE WITH SUBSTANTIAL VARIABILITY



- Must consider the impact of the variability
- Determine performance off design point
- Might have both supply and demand variability (as with electricity).
- There may be consequences for downstream (off-sun) processes to consider

COST DRIVERS ARE TECHNICAL METRICS IMPORTANT AT ALL PHASES OF DEVELOPMENT

- Total Project Investment or CAPEX: $Cx\ (\$/kW)$
- Capacity Factor: CF (Between 0 and 1)
- Energy Utilization: $eU\ (kWh/kg)$ $\propto$ 1/Efficiency
- Cost of energy plus variable O&M: $Ce\ \$/kWh$
- Annualized cost factor (financial plus fixed O&M): $crf\ \left(\frac{1}{yr}\right)$

$$\frac{\$}{kG_{Product}} = eU \times \left\{ \frac{Cx \times crf}{CF \times 8760\ hr/yr} + Ce \right\}$$

Power Density: kW/L
Measure of compactness

Balancing solar constraints and balance of system – won't necessarily eliminate cost of energy

May not match up on CF either

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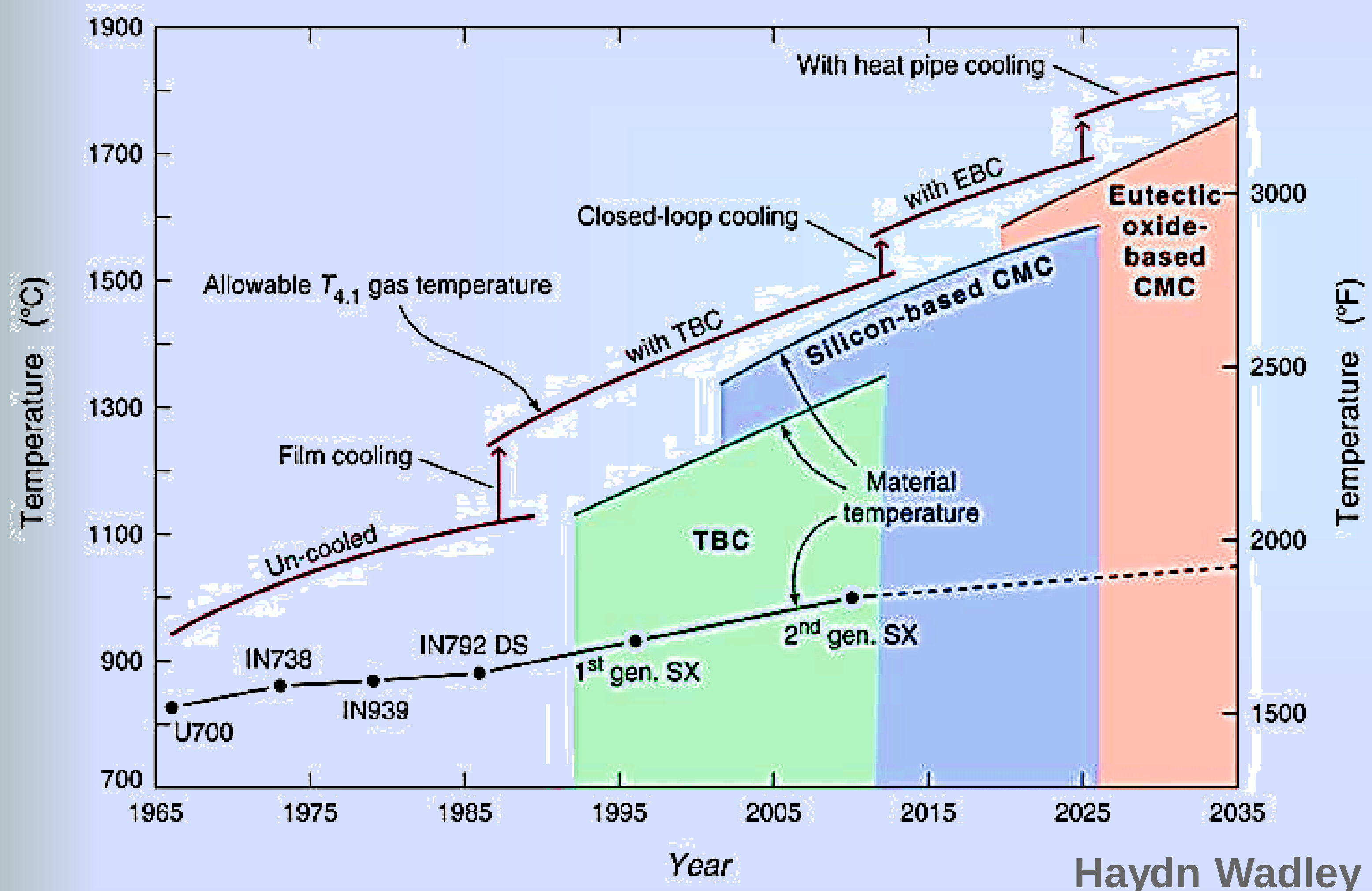
INLET TEMPERATURE ON JET ENGINES CONTINUOUSLY INCREASING



Haydn Wadley

The evolution of allowable gas temperature at the entry to the gas turbine and the contribution of superalloy development, film cooling technology, thermal barrier coatings and (in the future) ceramic matrix composite (CMC) air foils and perhaps novel cooling concepts.