Investigator
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Objective
The long-term objective of this research is to enable the widespread deployment of a new technology that converts sugars derived from cellulosic biomass into hydrogen, with energy conversion yields greater than 90% and fuel value conversions at volumetric productivities at least 10-fold higher than current U.S. biomass-to-ethanol technologies. The process for accomplishing this will use inexpensive bacterial cell extracts to convert glucose, xylose and water into hydrogen and CO₂. A kinetic and thermodynamic model for a novel, cell-free enzymatic pathway will be developed, providing new scientific insights.

Background
The U.S. market for hydrogen is very large and is likely to grow in coming decades. Hydrogen generated from methane is used to chemically reduce nitrogen gas – a crucial step in fertilizer production. The amount of carbon dioxide released is roughly equivalent to the CO₂ emitted from 34 million automobiles. The petrochemical industry also uses very large quantities of hydrogen, produced exclusively from fossil fuels with large releases of CO₂. If industrial hydrogen could be produced from cellulosic crops grown on marginal lands as well as cellulosic wastes from food crops, the resulting chemicals and ammonia fertilizers could be manufactured with minimal new CO₂ release. Using these raw materials would also avoid taking land away from food crops.

Approach
The proposed technology focuses on the pentose phosphate pathway – an important metabolic process in living cells (1, 2). This pathway is capable of fully converting glucose into CO₂, while generating 24 electrons in the form of 12 molecules of the coenzyme, NADPH, for each glucose molecule. Adding two additional enzymes can then produce 11 to 12 molecules of hydrogen (Figure 1).

To minimize cost, crude cell extracts containing high levels of the required enzymes will be used, including an iron-based hydrogenase that is at least 10 times faster at producing hydrogen than nickel-iron hydrogenases. This approach will circumvent the need for expensive protein purification steps.

Because the cells will no longer be alive, the extracts will be less sensitive to the toxins that are produced during the pretreatment and hydrolysis procedures that digest the cellulose to supply the sugars. A key goal is to demonstrate that crude cell extracts can satisfy the conversion efficiency and volumetric productivity goals.
Specific aims of the project include:

1. Develop a model of the NADPH-to-hydrogen-electron-transfer pathway that accurately predicts observed electron flux rates, while considering the influence of enzyme kinetics and thermodynamic driving forces. The model will be used to estimate optimal protein concentrations.

2. Use cellular debris and fluids to demonstrate hydrogen production from glucose with conversion efficiencies above 80% and rates above 100 kJ/liter-hour – double the rate for ethanol.

This approach uses a novel electron transfer pathway and couples this to crude cell extracts, another innovative technology. Because the project builds upon cellulose hydrolysis technologies that are being aggressively developed elsewhere, there is a reasonable expectation for a significant economic driving force to motivate large investments and widespread deployment at scale.

When successfully implemented, this technology has the potential to dramatically reduce CO$_2$ emissions by providing hydrogen as a chemical feedstock for nitrogen fertilizer production and for use in refineries and chemical production facilities. It also has the potential to supply fuel for electricity generation and other energy-intensive industries.

It is also likely that the existence of a nearly carbon neutral – or even carbon positive (if the CO$_2$ can be used) – large-scale and efficient hydrogen production technology will spur much more rapid development of improved hydrogen transportation and storage technologies. This, in turn, will allow even more widespread use of hydrogen as a clean, renewable fuel.

**References**
