Who We Are

The Adams research group at McMaster University is a leader in chemical engineering research that focuses on sustainable energy conversion systems, innovative chemical process design, and process systems engineering methodologies. We tackle major world issues related to chemical and energy systems, such as carbon dioxide capture, utilization and sequestration, power systems of the future, flexible chemicals production, mobile chemical technologies, synthetic fuels, alternative fuels, biofuels, renewable energy systems, nuclear energy, and many other areas of application. Prof. Adams’ team includes PhD students, masters students, undergraduates, full time research engineers and associates.

INDUSTRIAL COLLABORATIONS

Our research is driven by the triple bottom line of sustainability: economic sustainability, environmental sustainability, and socio-political sustainability. Our innovations and inventions must adhere to all three in order to make a real world impact. That is why we work closely with industry to focus on research that is most likely to be commercialized.

Industrial partners can get involved in a number of ways. Typically, industrial experts advise, collaborate, or participate in research activities directly on a project of mutual interest. Companies provide some funding to support basic research needs such as graduate student research stipends, computers, software, and licenses. Usually, industrial funding is leveraged by matching provincial or federal grants through various government programs.

The best way to get involved is by joining the McMaster Advanced Control Consortium (MACC). This is an industry-academe collaborative organization with 5 professors, over 20 students, and 7 companies. Research efforts are pooled for maximum research impact. Industrial partners are expected to participate in research activities for maximum impact. See macc.mcmaster.ca for more information.

CORE COMPETENCIES

- Process Systems Engineering
- Chemical Process Design and Process Synthesis
- Process Modeling & Simulation
- Process Optimization
- Process Dynamics
- Techno-Economic Analyses & Business Case Studies
- Life Cycle Analyses & Environmental Impacts
- Unit Operation Design

APPLICATION AREAS

- Industrial Energy Systems
- Gasification Technologies
- Coal / Petcoke / Biomass to Liquids and Fuels
- Gas to Liquids and Fuels
- Nuclear to Liquids and Fuels
- Advanced Power Plants
- CO₂ Capture Systems
- Mobile Chemical Plants
- Systems Standardization
- Integrated Community Energy
- Steel Refinery Off Gas Handling
- Solid Oxide Fuel Cells
- Power-to-X
- Energy Storage
- Energy Policy
- Agile & Flexible Chemical Manufacturing
- Semicontinuous Distillation
- Waste Rubber to Fuels
- Concentrated Solar Thermal Power

Our collaborators include 17 companies, universities, and government agencies.

Our alumni go on to major engineering companies, universities, and government agencies.

The Adams team has published 90 journal articles, books, and book chapters.

Key Honours and Awards

- University Scholar
- Canadian Journal of Chemical Engineering Lectureship Award
- CSChE Emerging Leader in Chemical Engineering Award
- Industrial & Engineering Chemistry Research’s 2018 Class of Influential Researchers
- Ontario Early Researcher Award
- Joseph Ip Distinguished Engineering Fellow

Key Positions and Memberships

- Section Editor-In-Chief, Processes (Computational Methods)
- Chair, Systems & Control Division, Canadian Society for Chemical Engineering
- Member, McMaster Advanced Controls Consortium
- Member, McMaster Institute for Energy Studies

Contact

Prof. Thomas A. Adams II
Associate Professor
Associate Chair (Graduate Program)
Department of Chemical Engineering

P.Eng. (Ontario)
PhD Chemical Eng. (U. Pennsylvania)
B.S. Chemical Eng. (Michigan State)
B.S. Computer Sci. (Michigan State)

http://macc.mcmaster.ca
Current Research Projects

The Adams group currently engages in many on-going research projects and thrusts. Here are some of our favorites.

STEEL REFINERY OFF GAS CONVERSION TO FUELS OR POWER

In this collaborative project with ArcelorMittal Dofasco in Hamilton, we are creating processes that reduce the CO\(_2\) footprint of steel refining through process retrofits which change how coke oven gas (COG) and blast furnace gas (BFG) are utilized. Currently, COG and BFG are used for low grade heat and for power production.

- **Option 1:** Retrofit the power system with a high efficiency combined cycle power system. We designed an advanced gas turbine based cycle that can be retrofitted into place without the need for heat substitution elsewhere in the plant, resulting in the same direct CO\(_2\) emissions but a higher power production, thus reducing net CO\(_2\) emissions from the grid.

- **Option 2:** Replace COG combustion with a process we designed that captures CO\(_2\) from the BFG and converts it to methanol, aided by advanced sulfur removal strategies. This both increases the potency of BFG for balance-of-plant uses and reduces direct CO\(_2\) emissions by “storing” carbon in methanol. Increased grid electricity and natural gas usage is required since COG is no longer combusted.

Our findings show that the best choices strongly depend on market prices, government carbon policy, and electric grid intensity. For example, Option 2 is better for the Hamilton refinery because grid emissions are so low, but Option 1 is better for a refinery in Finland because the carbon intensity is much higher.

GASIFICATION AND COOLING VIA METHANE REFORMING

This project involves the design of individual unit operations relating to methane reforming and included a collaboration with Imperial Oil. We have designed several devices which capture the heat from a high temperature gas (such as syngas from a downward entrained-flow gasifier or helium from a modular helium reactor) and use that to drive the endothermic methane reforming process. This is an excellent use of high temperature, high exergy heat which both provides syngas generation capabilities and gas cooling capabilities. It can be used with many kinds of solid fuels such as petcoke, cellulosic biomass, and coal. The reformer section can be designed for natural gas, methane, and even CO\(_2\) reforming as a CO\(_2\) sink.

This in turn enables the creation of new kinds of energy conversion systems. For example, biomass gasification can be used to make a carbon-rich syngas, and this device can be used to produce a hydrogen-rich syngas from natural gas and waste heat from the carbon-rich syngas. The two syngas streams can be blended to achieve the perfect carbon:hydrogen balance ideal for the production of methanol, Fischer-Tropsch gasoline and diesel, olefins, and many other chemicals and fuels.

Selected Publications

Selected Publications
Petroleum coke is produced as a waste from the refining of heavy crude oil, particularly Canadian crudes. Much of it is not useful except for combustion, which is not permitted in Canada because of its high carbon and other pollution impacts. So, it gets stockpiled as a waste. We are developing processes that convert waste petcoke into Fischer-Tropsch diesel and gasoline that can be blended into the refinery.

Our techno-economic analyses indicate that there can be a strong business case for the process from purely an economic perspective in many cases. It is also cost-competitive purely as a CO₂ mitigation strategy at cost-of-CO₂-avoided rates similar to biofuels. Our cradle-to-grave life cycle analysis indicated that it can also have a net reduction in CO₂ emissions when coupled with carbon capture and sequestration and used to displace conventional or oil-sands-derived fuels.

Above: This pet coke-to-liquids process produces drop-in synthetic gasoline and diesel from a synergistic combination of waste pet coke and natural gas, displacing petroleum and reducing supply-chain related environmental impacts. There is a business case for the process from a purely economic perspective, but also has an environmental case when carbon capture and sequestration is employed, with costs of CO₂ avoided comparable to biofuels. [7].

Right: The most environmentally friendly way to use pet coke in Canada is actually to ship (by rail) pet coke from Alberta refineries to Ontario, where it can be processed using low-carbon electricity. Wells-to-wheels life cycle analyses indicate it has lower impacts than conventional fuels in many areas [9].

Selected Publications

Semicontinuous distillation is an advanced form of distillation that has been developed and perfected by the Adams team over the past 15 years. The premise is that a single distillation column can be used to separate chemical mixtures that normally require two or three distillation columns to achieve. This is possible by the use of a complex design coupled with a custom control system that operates the column cyclically. Product is always withdrawn from the column, although in varying degrees throughout the cycle. Unlike batch though, there are no costly startup or shut-down phases in the cycle. The end result is a compact and cost effective system that is typically economically superior to traditional multicolumn designs at intermediate flow rates, especially those typical of biofuels and pharmaceutical manufacturing.

Selected Publications
Solid oxide fuel cells (SOFC) are an amazing power generation device that not only produces electricity at high efficiency but has many unique properties that can be exploited for benefits in the larger system. For over a decade, the Adams team has been developing SOFC systems at various scales ranging from building and community scale (~50 kW) to bulk municipal scale (~750 MW). They can be conveniently integrated with energy storage systems, air separation systems, and CO₂ capture systems.

SOFC systems are still largely pre-commercial, so we are currently collaborating with the US Department of Energy, Siemens, HCE Enregy, and other energy and utility companies to create systems that work well using existing technologies, rather than waiting for advances in materials and manufacturing to make cell lifetime improvements. Our main systems of interest include SOFC/gas turbine hybrids and integrated SOFC and electrolysis systems for energy storage capability. Our experimental SOFC lab is under construction at McMaster.

### Selected Publications


---

Energy storage is a major systems component of any municipal or neighbourhood power system, and will be even more important with the growth of renewable power systems and advanced baseload power systems like SOFCs. The Adams group has been developing models and algorithms that can create optimal system designs that factor in energy storage and market uncertainty. We have developed real time / rolling horizon optimization algorithms that re-run every few minutes that factor in both short and long term demand forecasting in order to make the best decisions on how to use our energy storage systems right now. Our research currently looks at energy storage systems such as compressed air energy storage, thermochemical energy storage (i.e. storage in high-energy chemical bonds), geothermal storage, phase change material storage, and others.

### Selected Publications


Above: Black lines are real electricity demands and red lines are the power produced by an SOFC system integrated with compressed air energy storage in Ontario market conditions. (A) Optimizing for load matching. (B) Optimizing for profit. [18]
Our most common type of collaboration is in the area of technology value assessments. Throughout the Adams research group, we typically use eco-techno-economic analysis and standardization techniques in order to evaluate the economic feasibility and environmental impacts of every new systems concept we put forward. We do this in order to understand our innovations in the context of the triple bottom line of sustainability. We also apply this for early technology screening of individual pieces of equipment. For example, our collaborators may have developed a new catalyst, membrane, reactor system, bioprocess, or separation technology. We then take that and try to assess its value by analyzing how the new technology would function in the context of the larger system. Typically, we need to design and simulate a new system that would incorporate the technology, and then use eco-techno-economic analyses to make judgements about the value of that technology compared to other competing strategies (which can result in similar or even very different systems).

Some example technology assessments we have or are conducting:

- Solvent screening for biobutanol extraction
- Advanced power plants w/ CO₂ capture
- Bio-butyl acrylate production
- Waste-to-succinic acid
- Seaweed as bio-feedstock
- Methanol to butanol conversion via acetic acid route
- Microwave-enhanced algal-derived lipid production
- Waste rubber-to-SNG

Above: Our technology assessment meta study for advanced (future) power systems with CO₂ capture technology. The study “de-hypes” the literature by recomputing key metrics such as life cycle greenhouse gas emissions and levelized cost of electricity (LCOE) according to a common set of analysis standards. This results in a clear and unbiased comparison between technologies, identifying the most and least promising for investment and research. [19]

MOBILE TECHNOLOGIES AND CHEMICAL PLANTS ON A TRUCK

One of the most exciting new areas within the field of chemical process design is in the area of modular, mobile, and portable systems. We have collaborated with Pioneer Energy (USA) and ChemBioPower (Alberta) to develop systems that can be deployed to oil & gas drilling sites (especially shale gas sites), pulp and paper mills, and remote northern communities on truck-mounted skids or in shipping containers. The goal is to capture waste energy from smaller, temporary sources like flare gas, locally harvested wood, or pulp and paper mill wastes and convert to useful products such as drop-in diesel substitutes on-site.

Adams group research has included the design of individual modules that can be mass-produced locally and deployed in shipping containers, the determination of optimal module deployment schedules and supply chain networks based on target markets, and the integration of deployed modules within a larger chemical processing network.

Selected Publications

Selected Publications
The Adams group has developed energy conversion systems of many kinds that use non-traditional energy sources, often in combination. This can provide both increased energy security by utilizing domestic feedstocks, and typically reduced environmental impacts compared to the status quo. We often design systems which combine different kinds of energy sources together (for example, biogenic carbon-rich biomass, hydrogen rich shale gas, and carbonless nuclear heat) in order to exploit synergies between them. Examples include:

- Nuclear-to-fuels systems which can produce transportation fuels with up to 20% energy content originating from uranium
- Biomass-gas-and-nuclear-to-diesel systems which produce transportation fuels with lower life cycle impacts than conventional diesel
- Shale-gas-to-olefins systems which use methanol as a convenient intermediate that links hundreds of shale gas sources to a centralized olefin production facility
- Biofuel production systems from switchgrass, wood, and seaweed through thermochemical routes
- Waste-rubber conversion to synthetic natural gas

**Selected Publications**


**FLEXIBLE POLYGENERATION AND AGILE CHEMICAL MANUFACTURING**

One major research focus in the Adams group is on flexible polygeneration, in which we create chemical plants which can change their product output mix based on market conditions. In this way chemical plants can be designed that are more robust in the face of market uncertainty and can respond to changing business or political circumstances. Our studies have shown that potentially up to an extra billion dollars in net present value can be earned in some cases by changing products along with prices and playing on the margins [30].

To do this, we combine chemical process synthesis and design expertise, process modeling and simulation, process intensification, techno-economic analyses, and optimization under uncertainty techniques. This simultaneously produces probability-based economically optimal designs and corresponding strategies for its operation once built depending on the market conditions of the moment. Business case analyses are used to compute the added-value of the flexibility compared to a single-product baseline.

**Selected Publications**


CARBON CAPTURE, UTILIZATION, AND SEQUESTRATION

Because the environmental aspect of the triple bottom line of sustainability is always a high priority concern, the Adams group develops better technologies for carbon capture, utilization, and sequestration (CCUS). Some example areas of interest are:

- Textbook chapter on solvent-based H2S and CO2 capture simulations
- Standardized technology value comparison between advanced power plant designs with carbon capture
- Invention of a new, highly efficient CO2 capture system for certain kinds of advanced power plants
- Techno-economic comparison of CO2 capture strategies for offshore power production applications
- The use of gas hydrates for ocean floor CO2 sequestration
- The design of reaction systems for CO2 utilization in mixed reforming systems using nuclear energy
- CO2 utilization from blast furnace gas for steel refinery applications
- CO2 capture and utilization for the food and beverage industry

Key Tools and Methods

In addition to engineering expertise and knowhow, we typically employ the following tools and methodologies:

**Modelling and Simulation**
- Aspen Plus
- Aspen Plus Dynamics
- Aspen Custom Modeller
- Aspen HySYS
- Aspen Energy Analyzer
- Aspen ProMV
- gProms
- Jacobian
- ProMax
- Pro/II
- In house / custom codes

**Optimization**
- GAMS
- Mathematical programming (NLP/MINLP etc.)
- Dynamic optimization / single shooting
- CasADi (for cyclic systems)
- Design under uncertainty techniques
- Particle swarm optimization

**Eco-Techno-Economic Analyses**
- Aspen Capital Cost Analyzer
- Present value / cash flow methods
- Business case analyses
- ISO 14040 compliant life cycle analyses
- ReCiPe / TRACI / GREET
- SimaPro
- OpenLCA
- Standardization and Standards Development

**Process Control**
- Integrated design and control
- Unit start-up
- Unit operation
- Cyclic systems

Selected Publications


Collaborators