

Application of multiphase reaction engineering and process intensification to the challenges of sustainable future energy and chemicals



Joseph B. Powell

Shell International Exploration & Production Inc., Shell Technology Center Houston, 3333 Highway 6 South, Houston, TX 77082, USA

HIGHLIGHTS

- Multiphase reaction engineering and process intensification are key tools for addressing future energy challenges.
- *A priori* prediction of reactor, catalyst, and separations-system performance can speed process development and deployment.
- Improved tools are needed for prediction of complex, multiphase and multicomponent systems, including trace chemistry.
- Laboratory reactor and pilot plant expertise remains an important skill for industry.

ARTICLE INFO

Article history:

Received 28 September 2015

Received in revised form

27 August 2016

Accepted 2 September 2016

Available online 7 September 2016

Keywords:

Multiphase reaction engineering

Process intensification

Scale-up

Multi-scale modeling

Process development

Future energy

ABSTRACT

Multiphase reaction engineering and process intensification can play a critical role in developing technologies to unlock the value and opportunities of shale gas, and to mitigate carbon footprints in providing sustainable options for future energy and chemicals. New and intensified reactor designs and separation systems will be essential for efficient methane conversion, biomass upgrading to fuels and chemicals, as well as for affordable carbon capture. The following review summarizes future energy challenges, and assesses the state of the art of chemical engineering science in providing the necessary tools for more rapid, efficient, and reliable technology development and scale up.

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1. Energy transition challenges

"Reaction engineering" is a key discipline to drive change in the conversion of energy resources into fuels and chemicals. The current high demand for this skill in industry is driven by increased opportunities to utilize methane as a feedstock for fuels and chemicals, resulting from the "shale gas" revolution (Yergin and Ineson, 2009; EIA, 2016a, 2016b), and the critical need to reduce net CO₂ and greenhouse gas emissions (IEA, 2015) while also increasing energy supply to meet growing global demand. Incremental improvements on existing technologies cannot accomplish these goals.

One characteristic of the current dilemma for energy and chemicals is the increasingly diverse array of future feed stocks and conversion technologies that will be required to simultaneously

achieve the goals for increased energy availability with reduced environmental footprint (Shell, 2013). Incorporating renewable energy sources such as biomass or solar power into the energy supply requires fundamentally new technology and infrastructure. Changes in the future energy portfolio are being driven by a projected global population increase from seven to more than ten billion by 2100, with much of the increase occurring in the developing world, and resulting in a net migration to cities (United Nations, 2015). Concerns over climate change are driving a need to reduce net fossil carbon emissions, despite a projected doubling in energy demand with rising wealth and population growth through 2100. Energy flows are connected to water usage and stewardship, as well as food production (Shell, 2013). The combined energy demand and sustainability drivers result in a need to process a wider variety of feed stocks and resources, from fossil to renewable, using more efficient and intensified designs. As reviewed by Chu and Majumdar (2012), the energy transition is also driving an

E-mail address: Joe.Powell@Shell.com

increased emphasis on renewable energy, with reaction engineering challenges in solar or wind energy storage, and conversion to molecular fuels using captured CO₂ or other energy carriers.

Fig. 1 presents one scenario for a global energy system in 2100 vs. today, for the energy transition required to mitigate the effect of carbon emissions on climate change (Shell, 2016). The transition will require reduction in emissions from current energy infrastructure and sources, in addition to the development of affordable ways to use, store, and generate fuels from renewable energy resources. Fig. 2 presents a scenario for carbon mitigation to achieve net zero emissions via this transition.

Among fossil feeds, hydraulic fracturing and horizontal drilling has led to a “shale revolution”, greatly enhancing production of natural gas, as well as natural gas liquids and tight oil (EIA, 2015; IEA, 2014). Abundant gas availability provides new incentives to convert methane to chemical building blocks such as ethylene and propylene or aromatic hydrocarbons, and to liquid gasoline and diesel fuels (Karakaya and Kee, 2016). Wood et al. (2012) review technologies for Gas-to-Liquids conversion via Fischer-Tropsch synthesis. New reactor designs are needed however to improve efficiency and reduce the carbon intensity of the conversion processes. A portion of the available gas is present in smaller

reservoirs or fields including offshore locations. Development of affordable modular systems for distributed production of fuels and chemicals to mitigate the need for flaring remains a target for efficient production of these resources. “Tight oil” or production of light liquid hydrocarbons also has been enhanced as a result of the shale revolution (Olsen, 2015; EIA, 2015; EIA, 2016a, 2016b), and provides new opportunities in hydrocarbon resource management and conversion.

2. Vision2020 and Demand for new multiphase reactor technology

A roadmap for Reaction Engineering was developed to support the chemical industry (Klipstein and Robinson, 2001) as part of an AIChE-sponsored workshop. Development of fundamentals-based kinetic and transport models, tools to facilitate multiphase reaction system scale-up, and systems integration tools to consider micro, meso, and macro scales, were considered as fundamental needs. Recent progress against these goals in multi-scale modeling and prediction has been provided in reviews by Dudukovic (2007, 2010), Dudukovic and Mills (2015), Charpentier (2002, 2016).

Given the enormous scale of the energy industry and its delivery infrastructure, the time and investment required to make a substantive change in its nature is also quite large. Incremental investment required to meet global energy and efficiency improvement demands to 2035 are estimated at \$48 trillion dollars (IEA, 2014). Decades are required to see a material change in energy infrastructure (Kramer and Haigh, 2009), as assets have a useful life well in excess of 20 years (EIA, 2015; IEA, 2014).

The diversity of feed stocks and new technologies required to change the energy mix and sequester carbon will challenge the chemical engineering community to find new ways to more rapidly develop and scale-up complex systems. A recent review by Degnan (2015) explores reaction engineering challenges in refining, where the combination of shale gas and oil plus heavy oil has created a bifurcation in feeds, with need for light paraffin upgrading and heavy oil conversion technologies. While methane itself is readily combusted for electrical power generation at reduced carbon footprint, conversion to chemical building blocks or to liquid fuels such as gasoline, diesel, or methanol and its derivatives can require high temperature endothermic (reductive) or exothermic (oxidative) coupling reactions, where selective conversion and heat transfer are major design issues. Lower-temperature routes through syngas require pre- or post-combustion separations from air to mitigate carbon footprint. Advanced integrated multiphase reactor designs (Harmsen and Chewter, 1999) and chemical looping systems (Fan et al. 2015) featuring integrated separations of hydrogen, oxygen, CO₂ and/or water are often required to obtain competitive economics.

Karakaya and Kee (2016), as well as Kee et al. (2016) describe reaction engineering challenges in the conversion of natural gas to fuels and chemicals. Methane conversion typically involves reaction temperatures in excess of 700 °C. Efficient generation of syngas for conversion to Fischer-Tropsch products or methanol represents one challenge for carbon footprint reduction. Direct or oxidative coupling of methane to olefin or aromatic products are both challenged by selectivity and yields (Holmen, 2009). Process intensification through use of microchannel (less than about one millimeter scale) reactors, and use of membrane reactors for combined reaction and separations, are approaches used to address heat transfer and thermodynamic constraints, and to potentially enable modularity for distributed production in smaller gas fields (Koortzen et al., 2014).

Capital efficiency is another consideration in use of natural gas resources. Liquefied natural gas (LNG) is supplied for utility gas

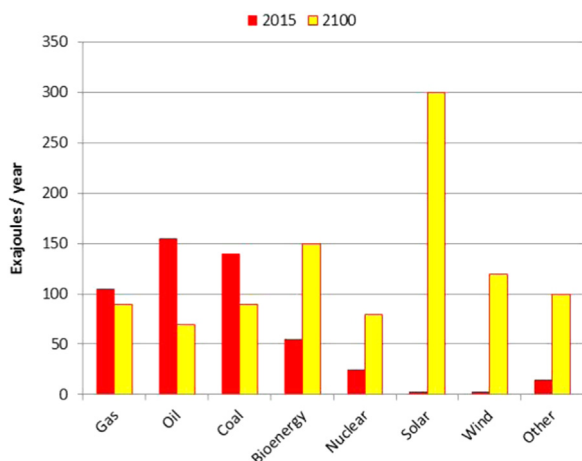


Fig. 1. Diversification of energy supply to address shale gas availability and mitigate climate change risk will drive an unprecedented pace of new technology innovation in energy and chemicals. Adapted from (Shell, 2016): A Better Life with a Healthy Planet, Pathways to Net-Zero Emissions, A New Lens Scenarios Supplement, p. 38.

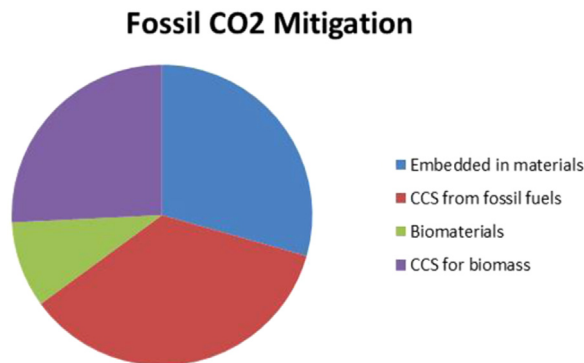


Fig. 2. Mitigation of greenhouse gas emissions can be achieved by embedding fossil and renewable (biomass) carbon into materials, as well as capture and sequestration of carbon dioxide. Adapted from (Shell, 2016), A Better Life with a Healthy Planet, Pathways to Net-Zero Emissions, a New Lens Scenarios Supplement, p. 69.

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