

A novel electric reactor for methane to acetylene conversion

Shauvik De¹, Alexander P. van Bavel², René Bos^{2*}

¹ Shell India Markets Private Limited, Bengaluru, Karnataka, India, 560103.

² Shell Global Solutions International B.V., P.O. Box 38000, 1030 BN Amsterdam, The Netherlands

*Corresponding author: rene.bos@shell.com

Highlights

- Introduction of a novel electrified reactor concept.
- Milli seconds flow through structured wire mesh at $T > 1500$ °C.
- CFD simulations to obtain an optimized reactor design.

1. Introduction

With renewable electricity becoming a highly widespread and accessible form of energy, electrification of chemical processes presents one of the most promising transition paths to low carbon footprint manufacturing of chemicals. A large number of chemical processes in industry are endothermic in nature and the required heat of reaction is provided by burning fossil fuels. The conversion of methane into acetylene has gained more attention in recent years and is one of the promising pathways to create acetylene and carbon black. This conversion is favorable at high temperatures (>1900 °C) and very low residence times (milli seconds or less), which is very challenging. The basic technology for acetylene production, using an electric arc reactor, has been around for many decades [1].

The current work introduces a reactor concept for high selectivity acetylene production where the required heat of reaction is provided directly via electricity, i.e. Joule heating, see also patent application [2]. The concept involves flow of a methane feed through a structured packing or arranged mesh or wire structures directly heated by green electricity, see Figure 1. Similar concepts have very recently been published for catalytic conversions, albeit for relatively low temperature applications [3-4]. For the much higher temperature methane to acetylene application, the concept also shows added advantages with respect to scale up, modularity and pressure drop compared to conventional reactor concepts for acetylene production.

It is the aim of this contribution to introduce the concept and provide an optimized design via detailed computational fluid dynamics (CFD) based numerical simulations.

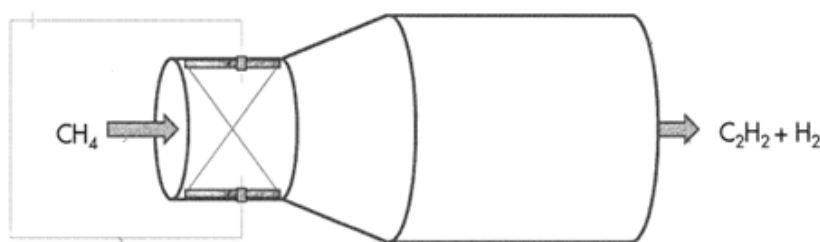


Figure 1. Schematic of electrified reactor concept [2]

2. Methods

To obtain the optimal design of the packing/wire structure a detailed high fidelity reactive CFD simulation was performed using the lumped kinetic model from the work of Holmen et al. [1]. A finite volume methodology was employed to solve the Navier stokes equation, using a commercial software package. Initially, only hydrodynamic simulations were performed using alternative mesh configurations to obtain the optimal mesh size, mesh configuration and pressure drop over such a mesh structure. Once those were obtained for a single mesh, simulations were performed for a series of these meshes including complex reaction kinetics and heat transfer phenomena.

3. Results and discussion

As shown in the work of Holmen et al. [1] and several other researchers, the conversion of methane to acetylene is favorable at very high temperatures (1500 – 2100 °C) and very low residence times, milli seconds. At lower temperatures (< 1500 °C) the selectivity towards acetylene decreases with increased coke formation. To obtain such a low residence time the flow through wire mesh configurations is designed as shown in Figure 2; the wire mesh diameter being in the millimeter range. The mesh can be directly heated with green electricity to provide the heat of reaction. The electric current flows through the mesh which heats up due to the resistive heating by employing a potential difference across the mesh.

Figure 3-a shows the temperature profile from the CFD simulations where the methane is fed at an inlet temperature of 600 °C and the residence time is set at 2 ms. Near the hot wire mesh the gas reaches the reaction temperature of around 2000 °C. Figures 3-b and 3-c show a high conversion of methane (>90 %) and production of acetylene with a selectivity significantly higher than conventional technologies.

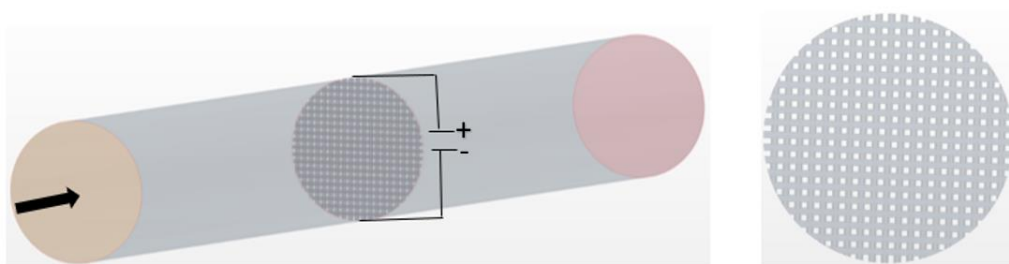


Figure 2. Wire meshed reactor configuration (the wire mesh is zoomed).

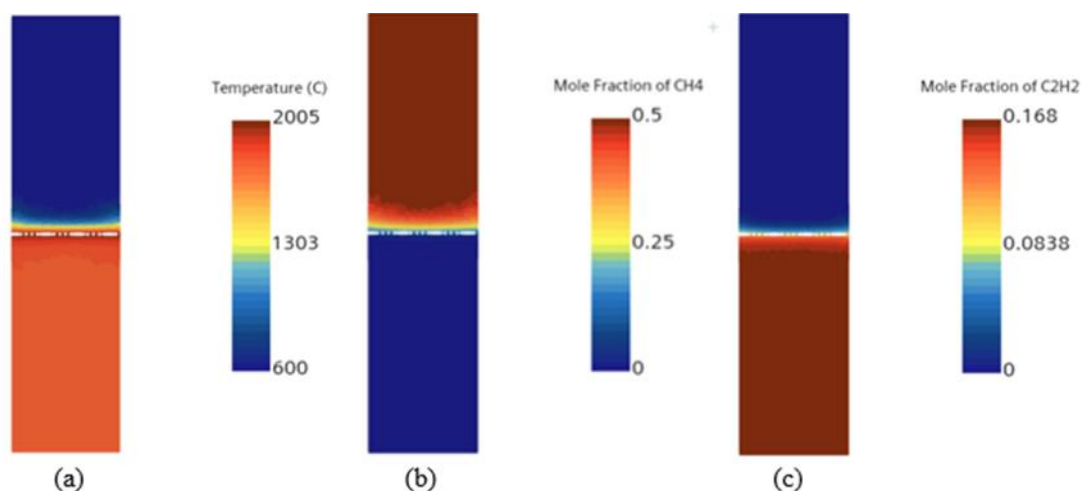


Figure 3. (a) Temperature profile in reactor (b) Methane and (c) Acetylene mole fractions

4. Conclusions

A novel electric reactor concept is proposed and evaluated for the high temperature and low residence time gas phase conversion of methane to acetylene. Simulations show the potential of such an electrified reactor as a greener and more sustainable technology for methane to acetylene production.

References

- [1] A. Holmen, O. A. Rokstad, A. Solbakken, *Ind. Eng. Chem. Proc. Des. Dev.*, 1976 15 (3), 439-444
- [2] S. De, A.P. van Bavel, European Patent; EP 3 845 513, 2020
- [3] L. Dou, C. Yan, L. Zhong, D. Zhang, J. Zhang, X. Li, L. Xiao, *Chem Commun*, 2020,**56**, 205-208
- [4] S.T. Wismann, J.S. Engbæk, S.B. Vendelbo, F.B. Bendixen, W.L. Eriksen, K. Aasberg-Petersen, C. Frandsen, I. Chorkendorff, P.M. Mortensen, *Science*, 2019 May 24;364(6442):756-759.

Keywords

Electric reactor, Methane conversion, Wire mesh, green technology.