



A fixed-bed reactor for energy storage in chemicals (E2C): Proof of concept

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HIGHLIGHTS

- A new type of fixed-bed reactor for steam-methane reforming.
- The application of electric resistance heating using the electrically conductive particles.
- A hybrid 3D-1D discrete heat transfer model.
- Electrical current distribution and amount of catalytic sites and interparticulate porosity.
- The optimal volume fraction of the catalyst is determined to be between 0.27 and 0.30.

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ABSTRACT

A new type of fixed-bed reactor for endothermic reforming, e.g. steam-methane reforming (SMR) or dry reforming of methane (DRM), is proposed. The reactor consists of two sorts of spherical particles: electrically conductive particles (large) and non-conductive catalyst particles (small). The main feature of this reactor is the application of electric resistance heating using the electrically conductive particles, which heat the non-conductive catalyst particles and reacting gas inside the reactor. In this work we consider a cylindrical fixed bed, which is 50 cm tall and has a bottom diameter of 10 cm, filled with electrically conductive particles made of nickel and with 1 cm in diameter. The open-source discrete-element method (DEM) software Yade is used to generate cylindrical fixed beds with binary dispersion. Steady-state particle temperatures are calculated based on a new 1D Euler - 3D Lagrange discrete heat transfer model that includes conduction between particles, forced convection and radiation. The design parameters of the fixed beds are calculated numerically based on the current distribution, temperature uniformity and amount of catalytic sites. The ideal catalyst radius is selected to be 0.4 of the radii of the conductive particles, based on the maximum radius at octahedral sites of closed packing. Analysis of simulations based on the electrical current and 3D temperature distribution revealed that the optimal volume fraction of the catalyst is determined to be between 0.27 and 0.30.

1. Introduction

The recent increase in the role of renewable energy in global final energy production is causing new challenges in the energy supply sector. In particular, to accommodate the mismatch between the energy demand and the supply of renewable sources (such as wind and sun) it is necessary to store the energy during production peaks [1]. Thus, the power network has to deal with great challenges not only transmission and distribution of electricity but also in terms of its storage. Electrical Energy Storage (EES) is now considered a key technology to establish renewables in mixed energy sources, e.g. see review [2]. This fact has intensified world-wide research and the development of important EES technologies including the operation principles, technical and economic performance features of different EES. A detailed analysis of real life

application and performance of the different energy storage (ES; electricity and heat) technologies was carried out by Aneke and Wang [3], featuring a comprehensive analysis of various energy storage projects all over the world. McKenna et al. [1] recently published a macro-economic analysis of the feasibility of Power-to-Gas (Power-to-Hydrogen, PtH) technologies in future. Using Baden-Württemberg as one of the leading industrial provinces in Germany, it was shown that rapid developments in the renewable energy sector will make it possible to have cost-covering PtH technologies after 2030 instead of 2040 as previously predicted.

One promising energy storage technology is the direct conversion of electrical current into chemical energy, which is called 'electricity to chemicals' (E2C), e.g. see reviews [4,2]. A well-known example of this type of conversion is the electrolysis of water to produce hydrogen,

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Nomenclature

\dot{E}_g	electrical heating power
ϵ_{cat}	fraction of catalysts with respect to total solid volume
I	current
U	electrical potential
S	shape factor of particle
R_p	electrical resistance of a single particle
R_{th}	thermal resistance of a single particle
ϕ	porosity of fixed bed
ψ	electric field potential
T_p	particle temperature
T_g	gas temperature
T_{nb}	neighboring particle temperature
h_{pg}	convective coefficient between particle and gas
r_p	particle radius
r_c	contact radius
d_i	particle diameter

d_{mean}	mean diameter of particles in the cross section
D	internal diameter of the reactor
N_p	number of electrically conduction particles in the cross section
ΔT_g	change in gas temperature
h_{pg}	particle-gas heat transfer coefficient
P	gas pressure
Nu	Nusselt number
Re	Reynolds number
Pr	Prantl number
A_p	Particle surface area

Physical constants

$T_{melting} = 1720$ K	melting point of Nickel solid particles
$E = 90$ GPa	Young's Modulus for solid particles
$\sigma = 5.67 \cdot 10^{-8}$ Wm ⁻² K ⁻⁴	Stefan-Boltzmann constant
$\epsilon = 0.9$	particle emissivity

where a direct electric current (DC) is used to drive a non-spontaneous chemical reaction, e.g. see the work [1] for a macroeconomic analysis of this type of energy storage. Alternatively, direct current (DC) can be used to heat any electrically conductive material (using the Joule heating effect) to 'sustain' the temperature for endothermic chemical reactions [5], e.g. CO₂ conversion into fuels [6].

One option to store electrical energy in chemicals is to use so-called steam methane reforming (SMR) and/or dry reforming of methane (DRM), which use endothermic reactions to convert CH₄ plus H₂O and CH₄ plus CO₂ into a syngas comprising CO and H₂, respectively. Steam-methane reformers (SMRs) have been commonly used to produce hydrogen [7,8] on an industrial scale. SMR is the conversion of methane to syngas, a mixture of carbon monoxide and hydrogen, using steam under a large heat supply due to the highly endothermic character of this process. Conventional industrial reactors use an array of radiant tubes filled with catalysts, and heat is supplied by a gas fire in the chamber outside the tubes or the heat comes from a solar dish system. Reformer tubes are typically heated to temperatures of 850–950 °C. For a comprehensive review of solar-based reformers, we refer to two excellent reviews [9,10]. During the dry reforming of methane, syngas and hydrogen are produced by methane reacting with carbon dioxide in the presence of a catalyst. Recently, this type of reforming has been extensively investigated due to the conversion of greenhouse gases (CO₂ and CH₄) into syngas, see reviews [11,12]. For a detailed review of a large number of different SMR/DRM reactor concepts we refer to the work [6].

One of the disadvantage in conventional reforming is the radial inhomogeneity of the temperature profile across the tube due to the fact that the heat is supplied to the gas and catalysts from the tube surface, e.g. see [13]. The nonhomogeneous distribution of temperature causes an uneven reaction rate, e.g. see the works [14,15]. In order to maintain a good temperature at the centre of the tube, the temperature of the radiant tube often far exceeds the reaction temperature, which compromises the thermal efficiency of the energy conversion [16], and up-scaling is a difficult task. To overcome this problem, the reactor can be heated using the Joule heating effect, supplied by a direct current flowing through a reactor. This concept was first introduced by Glaser and Thodos [5], who used the Joule heating effect to heat electrically conductive spherical particles packed randomly inside the cylinder. In particular, Glaser and Thodos [5] established experimental studies of heat and momentum by measuring the temperature and pressure of a gas flow through a fixed bed consisting of randomly packed metallic particles. Experiments have been conducted passing direct electrical current through the fixed bed consisting metal spheres to provide heat, which is continuously removed by the gas flow. Joule heating proved to

be effective when the fixed bed consists in conductive metal particles. Recently, Rieks et al. [6] introduced a novel electrically heated SMR/DRM reformer where heating elements, which have a wavy shape, are made from a FeCrAl alloy. The heating elements are coated with a LaNi_{0.95}Ru_{0.05}O₃ catalyst at different washcoat thicknesses. A combined operation of dry and steam reforming was investigated experimentally. The results showed a maximal CH₄ conversion of 29.4% using one heating element at 900 °C. It was possible to vary the H₂/CO ratio in the gas was between 0.4 and 12.3 by combining steam and dry reforming.

New developments in EES utilising reforming technologies are impossible without computer-based modeling. Recently, significant improvements in computational hardware (multi-processor-based desktop computers) and commercial CFD software (for example ANSYS-Fluent, COMSOL and STAR-CCM+) have made it possible to use computational fluid dynamics (CFD) to predict and scale up transport processes in reformers. SMR or DMR studied computationally using 1D, 2D or 3D models depending on the modeling purpose. Basically, 1D [17] and 2D [15,13] models apply a continuum approach approximating a fixed bed as a permeable porous media. In spite of their simplicity, such models show reasonable agreement with experimental data [13,14]. However, one of the main disadvantages of 1D and 2D simulations is a need for the spatial distribution of the volume fraction of solids across and along the reactor and dispersion coefficients [18]. Such distributions can be obtained using particle-resolved simulations employing CFD coupled with the discrete element method (DEM) or discrete particle method (DPM) [19,18,20]. The main idea of the discrete particle approach is to account for the geometric complexity of the packing structure using particle-resolved modeling of a packed bed geometrical topology with discrete particle sedimentation [21,20] or a Monte Carlo-based algorithm [18]. The coupled CFD-DEM approach allows fluid flows and transport properties to be modelled inside the bed, similarly to the in situ technique. Such simulations demand significant computing power and time [22], as a large number of control volumes are needed to resolve the particle surface and the void space between the particles. This is why particle-resolved CFD (PR-CFD) simulations, taking into account homogeneous and heterogeneous chemical reactions, are now restricted to small segments of the bed or to beds where the ratio between the tube diameter and the particle diameter is low; see recent review on progress in fixed-bed reactor modeling using particle-resolved CFD [20]. For example, Wehinger et al. [22] carried out detailed 3D CFD-based particle-resolved simulations of a tubular fixed bed for the catalytic dry reforming of methane consisting of 113 spherical solid particles in a tube with a diameter about 4 times greater than the particle diameter. A detailed surface mechanism for the dry reforming of methane was used, including 42 chemical reactions. The

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