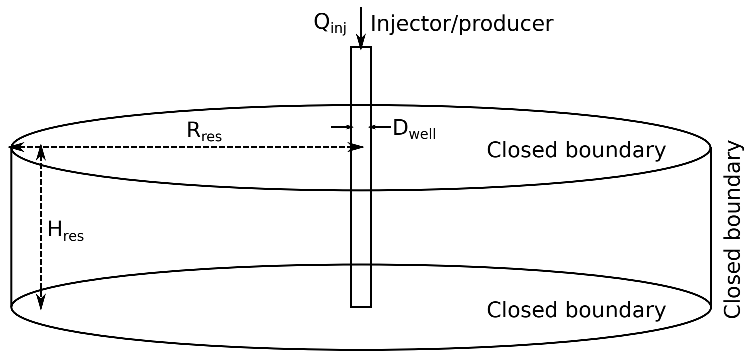

Figure 1: A cylindrical domain for the simulation of synthetic fuel storage in the subsurface

1 Problem formulation

Figure 1 shows a gas reservoir represented as a cylindrical domain. The top and bottom of the reservoir are closed, i.e. no flow, and the outskirt of the domain can either be closed or at hydrostatic pressure. The top side of the reservoir is located at depth L [m], the thickness of the reservoir is H_{res} [m] and the radius of the well and the reservoir are $0.5D_{well}$ and R_{res} [m] respectively. The permeability of the reservoir is k=10 mD [=10×10^{-12} m^2] and the porosity is φ=0.37. The reservoir is located close to an offshore windfarm and a surplus electricity of negligible price is provided to the operator to produce ammonia and store it in the subsurface. Ammonia is produced by a catalytic reaction between nitrogen and hydrogen:

$$N_2 + 3H_2 \rightarrow 2NH_3.$$

Nitrogen is separated from the atmosphere in a cryogenic air separation process and hydrogen is produced from the seawater in an electrolysis unit. All the separation and conversion is done offshore on the platform. There is no constant supply of electricity as the weather forecast gives the wind speed only a day in advance and the windfarm needs to provide electricity to the grid. The surplus electricity that is given to the ammonia production and storage fluctuates between 10 to 1000 MW.

2 Research questions and approach

The objective of this work is to calculate the energy loss in the process of producing, storing, and extracting ammonia as a synthetic fuel. The two main deliverable are

1. The energy efficiency of the process, i.e. chemical exergy of extracted ammonia divided by the total electricity consumption

2. The footprint of the process plant, i.e. the surface area (and weight of equipment) that the offshore platforms need to provide.

This problem will be addressed in two steps. First, the air separation, electrolysis, and ammonia synthesis processes will be simulated in Aspen Plus commercial process simulators. Depending on the limitations in the software and time restrictions, different levels of details will be included in the process models. These models are utilized to estimate the energy efficiency of the ammonia synthetic, i.e. the amount of electricity required to synthesize one unit mass of ammonia. The next step is the simulation of the subsurface storage and production. A simplified cylindrical reservoir model with a single well for the injection and production of ammonia will be created in COMSOL Multiphysics software with the boundary conditions described in Fig. 1. The reservoir is initially at hydrostatic pressure at a constant temperature of 70^{o}C and the concentration of ammonia in the reservoir is zero. The reservoir will be described by the single phase single component flow of an slightly compressible miscible fluid (ammonia) in the reservoir. The partial differential equations that describe the system are formulated in the next section.

3 Single phase flow formulation

The single phase compressible flow in porous media reads

$$\frac{\partial}{\partial t}\left(\varphi\rho\right)+\nabla.\left(\rho\mathbf{u}\right)=0,$$

where the Darcy velocity (assuming single phase flow and negligible gravity effect) and the fluid density are described as

$$\mathbf{u}=-\frac{k}{\mu}\nabla p,$$

$$\rho=\rho_0+\left(\frac{d\rho}{dp}\right)_{p_0}\left(p-p_0\right).$$

The flow of ammonia in the subsurface is described by

$$\frac{\partial}{\partial t}\left(\varphi c\right)+\nabla\left(\mathbf{u}c-\varphi\mathcal{D}\nabla c\right)=0.$$

In the above equations, φ [-] denotes porosity, k [m^2] denotes permeability, ρ [$\mathrm{kg/m}^3$] denotes the fluid density, p [Pa] denotes the reservoir pressure, μ [Pa.s] denotes the fluid viscosity, $\mathcal{D}$ [m^2/s] denotes the diffusivity of ammonia, and c [$\mathrm{mol/m}^3$] is the concentration of ammonia. Both viscosity and density are a function of ammonia concentration; however, we ignore this functionality in the preliminary model. The injection rate in the well is a function of the supplied electricity. We assume that for a week a constant power of 1 MW is provided for the synthesis of ammonia and in the following week, there is no supply of electricity (i.e. ammonia needs to be extracted from the reservoir). The pumping energy is calculated based on the calculated injection pressure in the well. Assume that the reservoir is initially filled with water and the ammonia and water are miscible.