# ASPEN Process Simulation for Ammonia Synthesis with A Catalytic Membrane Reactor Model Integrated Using MATLAB and Excel

Previously, we have successfully implemented a catalytic membrane reactor (CMR) model using MATLAB and evaluated the CMR's performance as functions of the operating conditions and membrane properties. However, to better design and optimize the CMR module, the reactor model has to be examined using the cost of ammonia production in the context of a process simulation.

ASPEN is widely used as the process simulation software. However, novel modules for process intensification such as the CMR are not predefined and cannot be simply replaced using a PBR and separator. ASPEN can allow the module customization in two ways. The first is to use a calculator module and write the associated FORTRAN code. Secondly, a user model can be defined in ASPEN which can be connected to Excel. Next, Excel can be used as a port to send and get data with MATLAB using the MATLAB-Excel add-in.

In this report, the second module customization method, a typical workflow from ASPEN to Excel and MATLAB will be discussed. The validity of the connection is verified against the tested CMR reactor model in MATLAB. The discussion will be in the context of implementing a CMR for an ammonia synthesis process.

# 1 Workflow

## 1.1 ASPEN module

A user-defined model (USER2) is used due to its capability to add multiple inlet and outlet streams. As shown in figure 1., the design parameters of CMRs are defined by specifying the integer and real parameters including the number of tubular CMRs, geometric properties including the length and radius of a tubular CMR, and the membrane properties including the ammonia permeance, nitrogen, and hydrogen selectivity.

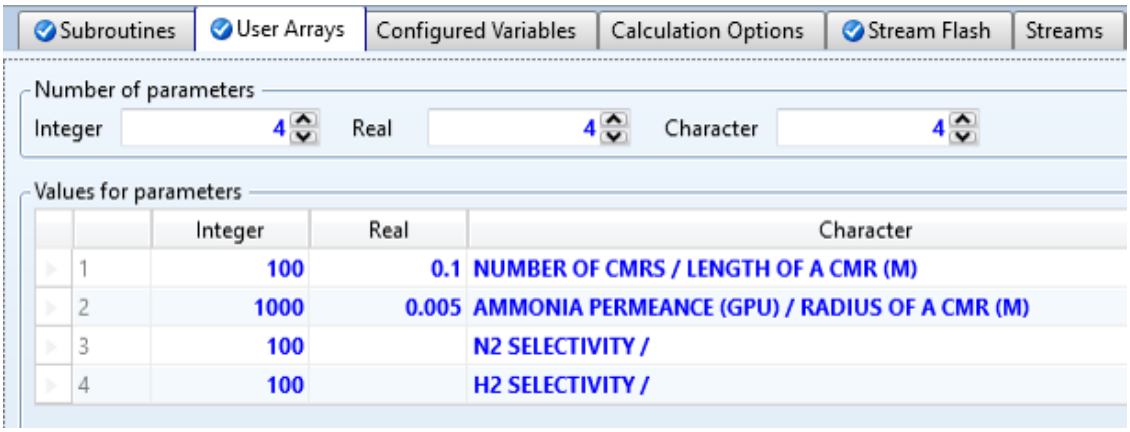


Figure 1: Setup of design parameters of the user model

ASPEN solves the process model using the sequential modular method. The reactor model requires the flow information of the inlet and sweep including temperature (T), pressure (P), total flow rate (Q), and composition (x). Then, the corresponding flow information of the permeate and retentate is calculated. Next, the stream flash option of the USER2 model uses the flow information (T, P, Q, and x) of the permeate and the retentate and calculates the associated thermo properties such as the molar entropy.

## 1.2 Excel connector

The ASPEN Excel connector used in this report is modified from the ASPEN user model manual [1] and Fonstalvo's work [2]. The former provides an example spreadsheet with built-in utility functions in macros to collect the ASPEN input and send the output back to ASPEN. The latter provides the utility macro which collects the Excel data, send the data and then retrieve the calculated results from MATLAB.

In the spreadsheet (ExcelASPENMatlabConnector.xlsm) attached, the tabs "Aspen_IntParams" and "Aspen_RealParams" correspond to the integer and real design parameters of the CMR from ASPEN, respectively. "Aspen_Input" contains the inlet flow information including the inlet and the sweep streams. The "Matlab" tab sends the input data to MATLAB and retrieves the calculated results. "Aspen_Output" represents the outlet flow information of the permeate and the retentate.

Table 1: The default units of flow properties

| Flow properties | Default units |
|---|---|
| Mole flow | kmol $s^{-1}$ |
| Temperature | K |
| Pressure | N $m^{-2}$ |

It is noted that for consistency ASPEN will convert the units of the data sent to Excel to the default ones (table 1) regardless of the user preference in the ASPEN model.

### 1.3 MATLAB model

The CMR model is written using MATLAB. Detailed information about the model can be found elsewhere (BenchmarkReactorModel.mlx). Notably, this model assumes the use of the ideal gas law, which might be different from the setup of the ASPEN model.

## 2 Testing and results

### 2.1 Comparison with the tested CMR model

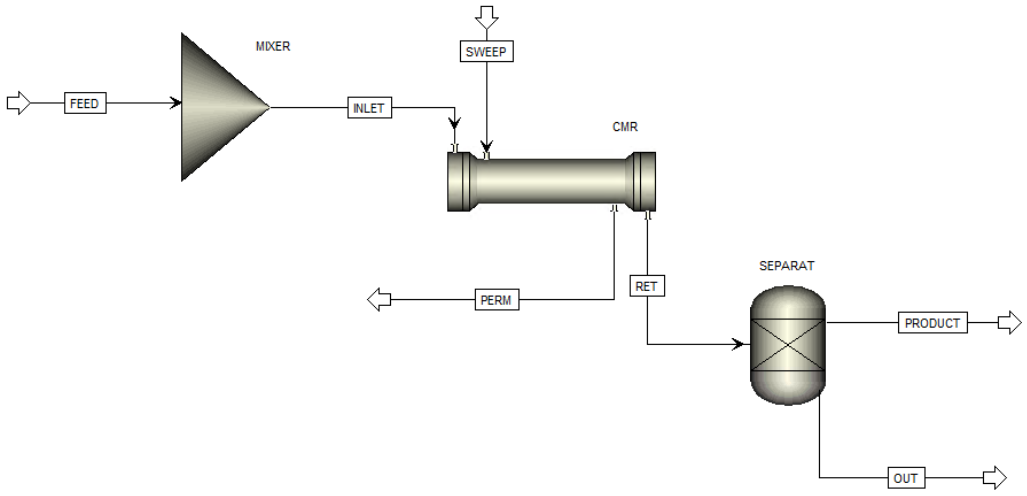


Figure 2: Process flow diagram of a CMR process for ammonia synthesis

Table 2: Flow setup of the feed and sweep streams

| Stream | Inlet | Sweep |
|---|---|---|
| $NH_3$ fraction | 0 | 0 |
| $N_2$ fraction | 0.25 | 1 |
| $H_2$ fraction | 0.75 | 0 |
| Flow rate (kmol s-1) | 7.45E-5 | 7.45E-8 |
| Temperature (K) | 723 | 723 |
| Pressure (bar) | 30 | 0.05 |

Table 3: Design parameters of the CMR

| | CMR parameters |
|---|---|
| Number of tubes | 100 |
| Length (m) | 0.1 |
| Radius (m) | 0.005 |
| Ammonia permeance (GPU) | 1000 |
| $N_2$ selectivity | 100 |
| $H_2$ selectivity | 100 |

Figure 2 shows an example of a CMR ammonia synthesis process. The feed stream is composed of stoichiometric $H_2$ and $N_2$. A sweep stream is used to create vacuum conditions on the permeate side. A separator is used to purify ammonia as the product stream. The out stream can be altered as a recycle stream connected to the mixer. Additional design parameters of the CMR and the operating conditions are summarized in the table 2 and table 3. The MATLAB model which has been tested separately is used to benchmark the performance of the process model. The comparison of the results of the retentate stream is summarized in table 4 showing the validation of the connection.

Table 4: Comparison of the retentate flow between MATLAB model and ASPEN simulation

| Retentate flow | MATLAB model | ASPEN simulation |
|---|---|---|
| $NH_3$ fraction | 0.036 | 0.036 |
| $N_2$ fraction | 0.241 | 0.241 |
| $H_2$ fraction | 0.723 | 0.723 |
| Flow rate (kmol $s^{-1}$) | 4.77E-5 | 4.77E-5 |

The mass balance of the CMR module is closed within 0.2% with a single pass. This deviation comes from two ways. First, the error is attributed to the truncation error between the conversion between kmol $s^{-1}$ to sccm. The former is used in the ASPEN model, whereas the latter is used in the MATLAB model. Second, the MATLAB model assumes the use of ideal gas law, which is different from the PENG-ROBINSON gas law used in the ASPEN simulation.

# References


[1] *Aspen Plus User Models*. Aspen Technology, Inc., 10 ed., 2020.

[2] J. Fontalvo, "Using user models in matlab® within the aspen plus® interface with an excel® link," *Ingeniería e Investigación*, vol. 34, no. 2, pp. 39–43, 2014.