Supporting Information: A two-step methodology for the selection and process optimization of Liquid Organic Hydrogen Carriers (LOHCs)

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1 General calculations for the LOHCs prescreening stage

1.1 Utilities estimation

In this section relevant information is included for the estimation of the utilities demand in the prescreening stage.

1.1.1 Intermediate temperature (t-cd) and pressure conditioning (p-cd)

The power demand for gas compression (W_{p-cd}) is obtained from Equation (S1), where (n_{p-cd}^{cp}) represents the number of compression stages, (F) the molar flow, (η_{cp}) the compressor yield and (k) the politropic constant. Then, (T_{p-cd}^{in}) represents the inlet temperature to each compressor. However, the first compressor may receive the gas from different conditions than the others. Hence, a feed temperature to the compressor train, (T_{p-cd}^{0}), is defined.

$$W_{p-cd} = \frac{(n_{p-cd}^{cp} - 1) F_{p-cd} R T_{p-cd}^{in}}{\eta_{cp}} \cdot \frac{k}{k-1} \cdot \left(r_{p-cd}^{(k-1)/k} - 1 \right) + \frac{F_{p-cd} R T_0}{\eta_{cp}} \cdot \frac{k}{k-1} \cdot \left(r_{p-cd}^{(k-1)/k} - 1 \right) \quad \text{(S1)}$$

The gases temperature after the first compressor ($T_{p-cd}^{fin'}$) and the subsequent outlet temperatures (T_{p-cd}^{fin}) are modelled trough Equation (S2). It allows to calculate the cooling demand ($Q_{p-cd}^{u_k}$) between stages in Equation (S3), where (C_p) represents the specific heat for each compound.

$$\begin{aligned} T_{p-cd}^{fin} &= T_{p-cd}^{in} \cdot \left(1 + \frac{1}{\eta_{cp}} \cdot \left(r_{p-cd}^{(k-1)/k} - 1 \right) \right) \\ T_{p-cd}^{fin'} &= T_{p-cd}^{0} \cdot \left(1 + \frac{1}{\eta_{cp}} \cdot \left(r_{p-cd}^{(k-1)/k} - 1 \right) \right) \end{aligned} \quad \text{(S2)}$$

$$Q_{p-cd}^{u_k} = (n_{p-cd}^{cp} - 2) \cdot \int_{T_{in}}^{T_{fin}} F_{p-cd} C_p dT + \int_{T_{in}}^{T_{fin'}} F_{p-cd} C_p dT \quad \text{(S3)}$$

The heating/cooling demands to adjust process stream conditions between other process operations (reaction, separations, storage), must be also accounted for in the calculations. The reactants/products temperature may need to be adjusted (T^{fin}_{t-cd}). Moreover, the change of phase of any of the compounds may be required. Hence, latent heat contribution (λ) must be included if there exist. If process streams are heated, the energy can be provided by several utilities (e.g., steam, hot oil, hot air) in different steps. The same way occurs if the stream demands from cooling (e.g, water, ammonia). The heat/refrigeration demand for each utility k (u_k) is denoted with ($Q^{u_k}_{t-cd}$) for each stage. A minimal temperature approach is considered for each utility. The bound is set by ($T^{u_k}_{max}$), which is the maximum achievable temperature by a heated/cooled stream without surpassing the minimum temperature difference. Preferably, a single utility ($Q^{u_1}_{t-cd}$) is used as shown in Equation (S4). However, in those cases where the system demands from other heating/cooling agents to avoid thermal crossover, a second ($Q^{u_2}_{t-cd}$), third ($Q^{u_3}_{t-cd}$) and so on utilities are considered (Equation (S5)). The phase change contribution is included in the calculations. For the sake of simplicity, it is introduced at a single utility range. To determine on which one, an average temperature is calculated based on compound fractions and single species boiling points.

$$Q^{u_1}_{t-cd} = F_{t-cd} \cdot \left(\int_{T^{in}_{t-cd}}^{T^{fin}_{t-cd}} C_p dT + \lambda \right) \tag{S4}$$

$$\begin{aligned} Q^{u_1}_{t-cd} &= F_{t-cd} \cdot \left(\int_{T^{in}_{t-cd}}^{T^{u_1}_{max}} C_p dT + \lambda \right) \\ Q^{u_2}_{t-cd} &= \int_{T^{u_1}_{max}}^{T^{u_2}_{max}} F_{t-cd} C_p dT \\ &\dots \\ Q^{u_n}_{t-cd} &= \int_{T^{u_{n-1}}_{max}}^{T^{fin}_{t-cd}} F_{t-cd} C_p dT \end{aligned} \tag{S5}$$

1.1.2 Reaction section (rs)

To calculate the energy demand of utility k for the reaction section ($Q^{u_k}_{rs}$), which is assumed to operate isothermally, Equation (S6) is used. There, (ΔH_r) represents the reaction enthalpy, (X) the reaction conversion and (F_{lc-rs}) the limiting compound of the reaction.

$$Q^{u_k}_{rs} = F_{lc-rs} X \Delta H_r \tag{S6}$$

1.1.3 Separation operations (sep)

In those separations involving non-volatile and volatile compounds or only volatile compounds, pressure and temperature conditioning considerations from previous sections are assumed. A flash separation stage and membrane technology are used respectively. In both cases, perfect component separation is assumed.

If the separation only involves non-volatile compounds, an atmospheric distillation is considered. To estimate the utility requirements for the condenser ($Q^{u_k}_{sep-cd}$), for the sake of simplicity, only the latent heat of the distillate (F_{D-dc}) is accounted for. It aims to avoid complex distillation models at this early stage. The energy requirements for the condenser are calculated trough Equation (S7), whereas the reboiler requirements ($Q^{u_k}_{sep-reb}$) are estimated based on Equation (S8). There, (F_{W-dc}) and (T_{W-dc}), represent the residue stream and its temperature, (F_{F-dc}) and (T_{F-dc}), the feed stream to the distillation column and its temperature and (T_{D-dc}) the temperature from the distillate.

$$-Q^{u_k}_{sep-cd} = F_{D-dc} \cdot \lambda \tag{S7}$$

$$Q^{u_k}_{sep-rb} = -Q^{u_k}_{sep-cd} + F_{D-dc} \cdot (T_{D-dc} - T_{ref}) + F_{W-dc} \cdot (T_{W-dc} - T_{ref}) - F_{F-dc} \cdot (T_{F-dc} - T_{ref}) \tag{S8}$$

1.2 Raw materials costs estimation

In order to estimate the raw material costs, the Table S1 is included with LOHCs, solvents and H_2 prices.

Table S1: Raw material prices.

Dibenzyltoluene (Niermann et al., 2019)	4.00 $/kg
Toluene (Niermann et al., 2019)	0.80 $/kg
Naphtalene (Niermann et al., 2019)	0.60 $/kg
N-ethylcarbazole (Uijthof et al., 2024)	2.60 $/kg
1,2-dimethylindole (LookChem, 2024)	2.00 $/kg
7-ethylindole (LookChem, 2024)	2.00 $/kg
Phenazine (Niermann et al., 2019)	26.00 $/kg
CO_2 (Niermann et al., 2019)	0.03 $/kg
1,2-dihydro-azaborine (Niermann et al., 2019)	100.00 $/kg
Dioxane (Book, 2024)	2.74 $/kg
Diglyme (Intratec, 2024)	0.55 $/kg
THF (Intratec, 2024)	2.50 $/kg
H_2 (Ball and Weeda, 2015)	4.00 $/kg

1.3 Considerations for the Fire and Explosion Index (F&EI) calculation

This section aims to include relevant assumptions and to complement the information included in the main document for the calculation of the F&EI (AIChE, 1994).

- The highest MF and NH from the compounds present at each process unit, are considered for each calculation.

- In order to calculate the penalties linked to chemical reaction, the guide refers to the endo and exothermicity of general reactions. A hydrogenation and a dehydrogenation takes place in each system. Therefore, in the case that the studied equipment involves a reaction, a normalization is done to show the differences between systems, as shown in Equations (S9) and (S10) for hydrogenation and dehydrogenation respectively. There, (ΔHr) and ($\overline{\Delta Hr}$) represent the reaction enthalpy for each system and the average reaction enthalpy for all the studied systems respectively. In the Dow's F&EI Guide hydrogenation receives a penalty of 0.3, and cracking (as dehydrogenation is not present in the guide), a penalty of 0.2.

$$Pen_{F_{1,1}} = 0.3 \cdot \frac{\Delta Hr}{\overline{\Delta Hr}} \tag{S9}$$

$$Pen_{F_{1,2}} = 0.2 \cdot \frac{\Delta Hr}{\overline{\Delta Hr}} \tag{S10}$$

- For the material handling and transfer penalty, hazard is only attributed to the flammable compounds storage. As a result, this contribution is only included in the calculations for storage units.

- The penalties attributed to enclosed and indoor units, access and drainage and spill control are neglected assuming that all eligible options comply the requirements to discard them. Similarly, since the process operates at or above atmospheric conditions and there not exist operations with low temperatures and low-size particles, the penalties referred to sub-atmospheric pressure, dust explosion and low temperature are neither considered.

- In the case of penalties linked to the operation near or in the flammable range, only those contributors attributed to equipment failure events are considered.

- The penalty referred to the relief pressure is only applied to those units operating above atmospheric pressure. For its calculation, the relief pressure is assumed to be 25% higher than the operating pressure.

- To quantify the flammable material for each operation two contributors are considered: species in the process and compounds stored. To account for the species in the process, this contribution is assumed negligible for units such as heat exchangers or separators. However, reactors may present considerable residence times. Hence, average reaction times are considered to calculate the species in the process. These are: 1 h residence time for hydrogenation and 3 h for dehydrogenation according to the kinetics for some of the LOHCs of study (Dong et al., 2019; Chen et al., 2018). Then, to set the process capacity, the results from Eypasch et al. (2017) are taken into account. The storage of 6500 MWh is considered to be used during 20 days with a 39% electrical efficiency. With regards to the contribution of stored compounds, it is only applied to the storage tanks. To estimate the quantity of hydro and dehydrogenated LOHCs and the required solvents at each tank, a 1000 MWh energy storage in the form of hydrogen is considered in all cases assuming a split of the total storage capacity.

- As long as hydrogen is present in some equipment, corrosion phenomena is very likely. Hence, according to the Dow's F&EI Guide, a medium corrosion rate and stress corrosion (hydrogen embrittlement is not defined in the guide) are included in those operations where hydrogen exists. Furthermore, an additional penalty referred to regular leakage is also included.

- In those LOHCs systems in which hot oil is demanded as utility, a penalty is applied based on the quantity of hot oil released from the heating system. To estimate it, the hot oil demand for each process during a time lapse of 15 min is considered as the guide refers to the hazard of a spill for that period.
- The penalties referred to rotating equipment and the use of fired equipment are discarded. For the former, it is assumed that the power requirements of pumps and compressors do not surpass the threshold proposed in the Dow's F&EI Guide. With regards to the fired equipment, the distances to other equipment units are assumed long enough to discard any penalty.

2 Hydrogenation and dehydrogenation processes detailed formulation

2.1 Mixers and splitters

The mass and energy balances are performed for each mixer and splitter in Equations (S11) and (S12). There, (F) represents the molar flow and (H) the enthalpy for each stream. The inlet and outlet streams are denoted with the subindexes i and j respectively and each component with the subindex c. Furthermore, the operating pressure (P) is set equal for all inlet and outlet streams, whereas the temperature (T), and the composition (x) for all the outlet streams.

$$\sum_{i}^{I} F_{i,c} = \sum_{j}^{J} F_{j,c} \tag{S11}$$

$$\sum_{i}^{I} H_{i} = \sum_{j}^{J} H_{j} \tag{S12}$$

$$T_{j=1} = T_{j=2} = ... = T_{j=J-1} = T_{j=J} \tag{S13}$$

$$P_{j=1} = P_{j=2} = ... = P_{j=J-1} = P_{j=J} = P_{i=1} = P_{i=2} = ... = P_{i=I-1} = P_{i=I} \tag{S14}$$

$$x_{j=1,c} = x_{j=2,c} = ... = x_{j=J-1,c} = x_{j=J,c} \tag{S15}$$

2.2 Heat exchangers

The mass and energy balances for each heat exchanger are modelled according to the Equations (S16-S18). The hot and cold side are denoted with hs and cs indexes, whereas the inlet and outlet streams for each side are represented with IN and OUT respectively. The heat demand (Q) is calculated based on the differences of enthalpy. Furthermore, to estimate the heat exchange area (A) for each unit, the logarithmic temperature difference (Δ T_{log}) and the overall heat transfer coefficient (U) are considered as shown in Equation (S19). Typical U values are taken from Sinnott and Towler (2020b) for each heat exchanger based on the fluids circulating on each side.

$$F_{hs,IN,c} = F_{hs,OUT,c} \tag{S16}$$

$$F_{cs,IN,c} = F_{cs,OUT,c} \tag{S17}$$

$$H_{cs,OUT} - H_{cs,IN} = H_{hs,IN} - H_{hs,OUT} = Q \tag{S18}$$

$$Q = UA\Delta T_{log} \tag{S19}$$

$$P_{cs,IN} = P_{cs,OUT} \tag{S20}$$

$$P_{hs,IN} = P_{hs,OUT} \tag{S21}$$

$$T_{cs,IN} \leq T_{cs,OUT} \tag{S22}$$

$$T_{hs,IN} \geq T_{hs,OUT} \tag{S23}$$

2.3 Flash separation vessels

The mass and energy balances for flash vessels are included in Equations (S24) and (S25). These units receive a gas-liquid stream and separate both phases. Equilibria conditions are considered between gas (g) and liquid (l). Therefore, the outlet temperatures (Equation (S26)) and pressures (Equation (S27)) are equal. Moreover, no pressure drop is considered on this unit. To describe the equilibrium conditions for each component, the vapor pressure (P_v) is taken for the LOHCs (Equation (S28)), whereas Henry coefficient (He) is considered for the hydrogen (Equation (S29)). To set the dimensions for the flash vessel, the maximum allowable gas velocity is calculated from Sinnott and Towler (2020a) for an horizontal unit with mist eliminator. From the same reference, a minimum 10 minutes residence time is considered for the liquid, an aspect ratio of 4 is set and the liquid level is expected to cover the half of the transversal area.

$$\sum_{i}^{I} F_{i,c} = \sum_{j}^{J} F_{j,c} \tag{S24}$$

$$\sum_{i}^{I} H_{i} = \sum_{j}^{J} H_{j} \tag{S25}$$

$$T_{j=1} = T_{j=2} \tag{S26}$$

$$P_{i=1} = P_{j=1} = P_{j=2} \tag{S27}$$

$$P_{v,c} \cdot x_{l,c} = P \cdot x_{g,c} \tag{S28}$$

$$He_{c} \cdot x_{l,c} = P \cdot x_{g,c} \tag{S29}$$

2.4 Valves

The mass balance to valves is based in Equation (S30). It is assumed that the pressure drop on them (S31) do not originate a change in the temperature for liquids as shown in Equation (S32). Differently, for a gaseous stream, the change of temperature with pressure is characterized by the Joule-Thomson coefficient (μ_{JT}) (Equation (S33)).

$$F_{IN,c} = F_{OUT,c} \tag{S30}$$

$$P_{IN} \geq P_{OUT} \tag{S31}$$

$$T_{IN} = T_{OUT} \tag{S32}$$

$$T_{OUT} = T_{IN} + \mu_{JT} \cdot \Delta P \tag{S33}$$

2.5 Compressors

The compressors units must avoid the presence of liquid phase in the inlet stream. Therefore, previous to the compressor itself, a knockout flash vessel is placed in order to remove it, in case there exist. The Equation (S34) represents the separation between gas and liquid phases and Equation (S35) accounts for the energy balance to this previous stage to the compressor. Then, the gas-liquid equilibria is modelled as done previously in Equations (S28) and (S29). The flash stage is assumed to be isobaric and the outlet pressures (Equation (S37)) and temperatures (Equation(S36)) are equal as a result of the equilibria.

$$F_{IN,c} = F_{IN,c,g} + F_{IN,c,l} \tag{S34}$$

$$H_{IN} = H_{IN,g} + H_{IN,l} \tag{S35}$$

$$T_{IN,g} = T_{IN,l} \tag{S36}$$

$$P_{IN} = P_{IN,g} = P_{IN,l} \tag{S37}$$

After the removal of the liquid phase, the compression of the gaseous one is performed. The mass balance to this stage is presented in Equation (S38). The power demand for this step (W_{cp}) is modelled trough Equation (S39) assuming a politropic behavior for the gas. For that, the politropic yield (η_{cp}) and politropic constant (k) are taken as 0.75 and 1.4 respectively (Couper et al., 2005). The compression ratio (r_{cp}), defined in Equation (S40), is set between 1 and 4. Then, the temperature increase is modelled according to Equation (S41).

$$F_{IN,c,g} = F_{OUT,c,g} \tag{S38}$$

$$W_{cp} = \frac{\sum_c^C F_{IN,c,g} \cdot RT_{in,g}}{\eta_{cp}} \cdot \frac{k}{k-1} \cdot \left(r_p^{\frac{k}{k-1}} - 1 \right) \tag{S39}$$

$$1 \leq r_p = \frac{P_{OUT,g}}{P_{IN,g}} \leq 4 \tag{S40}$$

$$T_{OUT,g} = T_{IN,g} \cdot \left(1 + \frac{\left(\left(r_p^{\frac{k}{k-1}} - 1 \right) \right)}{\eta_{cp}} \right) \tag{S41}$$

2.6 Pumps

The mass balance to each pump is included in Equation (S42). In order to estimate its power consumption (W_{pump}), the Equation (S43) is applied. There, (η_{pump}) and ($\dot{V}$) represent the pump efficiency and the volumetric flow respectively. The former is set to 0.75 (Couper et al., 2005). Finally, this unit is assumed isothermal (Equation(S45)).

$$F_{IN,c} = F_{OUT,c} \tag{S42}$$

$$W_{pump} = \frac{\dot{V} \cdot (P_{OUT} - P_{IN})}{\eta_{pump}} \tag{S43}$$

$$P_{IN} \leq P_{OUT} \tag{S44}$$

$$T_{IN} = T_{OUT} \tag{S45}$$

2.7 Hydrogenation reactors

For the hydrogenation reactors, previous work is considered for the modelling (Prieto et al., 2023). On it, a detailed 1-D formulation, considering mass, heat and momentum transfer, with differential and highly non-linear equations is presented. Then, a series of surrogate models were developed to obtain more simple expressions to be used in other applications. Hence, the use of these simplified models is possible for the LOHCs process modelling. In the case of indoles mixture system, the surrogate models were already obtained from this previous work. Hence, these were used. However, the N-ethylcarbazole system has not been assessed yet. Therefore, following the same approach, a series of surrogate models were developed to model the hydrogenation reactors for this system. The same 1-D formulation was used to describe mass, heat and momentum transfer on these reactors. However, different kinetics are introduced. For the N-ethylcarbazole hydrogenation Wan et al. (2013) work was used to include the intrinsic kinetics in the reactor modelling. Note that the presence of four compounds is reported: the fully hydrogenated (NEC-12H) and dehydrogenated (NEC-0H) species and two reaction intermediates (NEC-8H) and (NEC-4H). However, the concentrations of these two last species are considerably lower compared to the other compounds at higher conversions (Huang et al., 2023). Therefore, it is assumed that the final concentration of both is zero after the hydrogenation reaction.

2.7.1 Slurry reactors

The Equation (S46) is included to model the hydrogenation conversion in a slurry reactor for the NEC system. There, (D), (V_{sl}) and (C_{sl}) refer to reactor diameter, slurry phase volume and catalyst concentration in the slurry phase. Moreover, ($u_{g,0}$) refers to the superficial gas velocity.

$$\frac{F_{in,EC0} + F_{in,EC4} \cdot 8/12 + F_{in,EC8} \cdot 4/12 - (F_{out,EC0} + F_{out,EC4} \cdot 8/12 + F_{out,EC8} \cdot 4/12)}{F_{in,EC0} + F_{in,EC4} \cdot 8/12 + F_{in,EC8} \cdot 4/12} =$$
$$- 2.80 \cdot 10^{-2} \cdot T - 1.03 \cdot D + 2.68 \cdot 10^{-2} \cdot C_{sl} + 1.58 \cdot 10^{1} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12))$$
$$+ 7.07 \cdot 10^{-2} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) + 5.49 \cdot 10^{-2} \cdot P - 6.33 \cdot u_{g,0}$$
$$+ 1.09 \cdot 10^{-1} \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) + 5.98 \cdot 10^{-5} \cdot T^2 + 1.13 \cdot 10^{-1} \cdot D^2$$
$$- 1.44 \cdot 10^{-5} \cdot C_{sl}^2 + 2.70 \cdot 10^{1} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12))^2$$
$$- 1.27 \cdot 10^{-2} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)^2 - 8.59 \cdot 10^{-5} \cdot P^2 + 1.38 \cdot 10^{-1} \cdot u_{g,0}^2$$
$$- 1.72 \cdot 10^{-4} \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)^2 + 9.81 \cdot 10^{-4} \cdot T \cdot D - 4.60 \cdot 10^{-5} \cdot T \cdot C_{sl}$$
$$- 2.45 \cdot 10^{-2} \cdot T \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)) - 7.01 \cdot 10^{-4} \cdot T \cdot V_{sl}$$
$$- 8.13 \cdot 10^{-5} \cdot T \cdot P + 9.37 \cdot 10^{-3} \cdot T \cdot u_{g,0} - 1.57 \cdot 10^{-4} \cdot T \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$- 1.40 \cdot D \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)) + 8.71 \cdot 10^{-2} \cdot D \cdot V_{sl} + 3.21 \cdot 10^{-3} \cdot D \cdot P$$
$$+ 1.58 \cdot D \cdot u_{g,0} - 1.65 \cdot 10^{-3} \cdot D \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$- 9.07 \cdot 10^{-5} \cdot C_{sl} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) - 2.29 \cdot 10^{-4} \cdot C_{sl} \cdot V_{sl} - 2.92 \cdot 10^{-5} \cdot C_{sl} \cdot P$$
$$+ 6.62 \cdot 10^{-4} \cdot C_{sl} \cdot u_{g,0} - 2.54 \cdot 10^{-6} \cdot C_{sl} \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$- 1.63 \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)) \cdot V_{sl} - 4.32 \cdot 10^{-2} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)) \cdot P$$
$$- 7.19 \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)) \cdot u_{g,0}$$
$$+ 4.97 \cdot 10^{-2} \cdot V_{sl} - 3.72 \cdot 10^{-3} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) \cdot V_{sl}$$
$$+ 1.58 \cdot 10^{-2} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) \cdot u_{g,0}$$
$$- 2.14 \cdot 10^{-4} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$+ 3.72 \cdot 10^{-4} \cdot V_{sl} \cdot P + 5.26 \cdot 10^{-1} \cdot V_{sl} \cdot u_{g,0} + 3.40 \cdot 10^{-4} \cdot V_{sl} \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$+ 1.64 \cdot 10^{-2} \cdot P \cdot u_{g,0} - 1.59 \cdot 10^{-4} \cdot P \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right)$$
$$- 7.43 \cdot 10^{-3} \cdot u_{g,0} \cdot \left(\frac{V_{sl}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)}\right) \tag{S46}$$

2.7.2 Trickle bed reactors

The hydrogenation conversion in trickle bed reactors for the NEC system is modelled trough Equation (S47). There, (L_{in}) and (G_{in}) account for the inlet liquid and gas flowrates and (W_{cat}) for the catalyst weight used in the reactor.

$$\frac{F_{in,EC0} + F_{in,EC4} \cdot 8/12 + F_{in,EC8} \cdot 4/12 - (F_{out,EC0} + F_{out,EC4} \cdot 8/12 + F_{out,EC8} \cdot 4/12)}{F_{in,EC0} + F_{in,EC4} \cdot 8/12 + F_{in,EC8} \cdot 4/12} =$$
$$\begin{aligned}
&7.61 \cdot 10^{-3} \cdot T_{in} - 1.75 \cdot D - 1.11 \cdot 10^{-1} \cdot L_{in} + 5.80 \cdot 10^{-2} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) \\
&+ 2.66 \cdot 10^{-2} \cdot P_{in} + 3.85 \cdot 10^{-4} \cdot W_{cat} - 2.07 \cdot 10^{-1} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12)) \\
&+ 9.95 \cdot 10^{-7} \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) + 9.96 \cdot 10^{1} \cdot \frac{1}{W_{cat}} + 4.37 \cdot 10^{-1} \cdot D^2 \\
&+ 4.53 \cdot 10^{-3} \cdot L_{in}^2 - 5.52 \cdot 10^{-1} \cdot G_{in}^2 - 1.88 \cdot 10^{-3} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right)^2 \\
&- 7.75 \cdot 10^{-5} \cdot P_{in}^2 - 6.90 \cdot 10^{-9} \cdot W_{cat}^2 - 1.48 \cdot 10^{2} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12))^2 \\
&+ 6.71 \cdot 10^{-14} \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right)^2 + 4.44 \cdot 10^{3} \cdot \left(\frac{1}{W_{cat}} \right)^2 - 1.12 \cdot 10^{-4} \cdot T_{in} \cdot L_{in} \\
&+ 1.33 \cdot 10^{-4} \cdot T_{in} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 2.51 \cdot 10^{-5} \cdot T_{in} \cdot P_{in} \\
&- 3.27 \cdot 10^{-9} \cdot T_{in} \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 1.21 \cdot 10^{-1} \cdot T_{in} \cdot \frac{1}{W_{cat}} - 3.06 \cdot 10^{-1} \cdot D \cdot G_{in} \\
&- 8.11 \cdot 10^{-5} \cdot D \cdot W_{cat} - 3.16 \cdot D \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12)) \\
&- 2.66 \cdot 10^{-7} \cdot D \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 4.42 \cdot 10^{2} \cdot D \cdot \frac{1}{W_{cat}} \\
&- 8.80 \cdot 10^{-4} \cdot L_{in} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 1.04 \cdot 10^{-4} \cdot L_{in} \cdot P_{in} + 1.26 \cdot 10^{-6} \cdot L_{in} \cdot W_{cat} \\
&- 1.98 \cdot 10^{-3} \cdot G_{in} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) + 6.19 \cdot 10^{-3} \cdot G_{in} \cdot P_{in} + 2.03 \cdot 10^{-5} \cdot G_{in} \cdot W_{cat} \\
&+ 3.34 \cdot 10^{1} \cdot G_{in} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12)) \\
&+ 7.90 \cdot 10^{-5} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) \cdot P_{in} \\
&- 1.05 \cdot 10^{-6} \cdot \left(\frac{F_{in,EC12} + F_{in,EC8} \cdot (8/12) + F_{in,EC4} \cdot (4/12)}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) \cdot W_{cat} - 1.71 \cdot 10^{-7} \cdot P_{in} \cdot W_{cat} \\
&- 2.94 \cdot 10^{-9} \cdot P_{in} \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 1.92 \cdot 10^{-1} \cdot P_{in} \cdot \frac{1}{W_{cat}} \\
&- 9.39 \cdot 10^{-4} \cdot W_{cat} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12)) \\
&+ 2.08 \cdot 10^{-11} \cdot W_{cat} \cdot \left(\frac{W_{cat}}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right) - 1.28 \\
&+ 3.02 \cdot 10^{4} \cdot (F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC4} \cdot (4/12)) \cdot \frac{1}{W_{cat}} \\
&- 8.22 \cdot 10^{-5} \cdot \left(\frac{1}{F_{in,EC0} + F_{in,EC4} \cdot (8/12) + F_{in,EC8} \cdot (4/12)} \right)
\end{aligned} \tag{S47}$$

2.8 Dehydrogenation reactors

Likewise for the hydrogenation reactors, a series of surrogate models were developed for the NEC system dehydrogenation following the same approach as in Prieto et al. (2023). For that, the dehydrogenation kinetics from Dong et al. (2016) are considered. Note also, that in this case, the presence of intermediate species is not neglected.

2.8.1 Slurry reactors

The dehydrogenation yields in slurry reactors for the NEC system compounds are modelled trough Equations (S48-S50).

$$\frac{F_{out,EC0}}{F_{in,EC12}+F_{in,EC8}+F_{in,EC4}+F_{in,EC0}} = -2.46\cdot10^{-3}\cdot T + 3.66\cdot10^{-3}\cdot C_{sl} - 4.36\cdot10^{1}\cdot F_{in,EC12} + 5.17\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}$$
$$+ 2.95\cdot10^{-2}\cdot V_{sl} - 5.64\cdot10^{1}\cdot F_{in,EC8} - 1.20\cdot10^{1}\cdot F_{in,EC4} + 1.42\cdot10^{-5}\cdot\frac{V_{sl}}{F_{in,EC12}} - 1.62\cdot10^{-5}\cdot V_{sl}\cdot C_{sl}$$
$$+ 7.76\cdot10^{-6}\cdot T^2 - 1.22\cdot10^{-6}\cdot C_{sl}^2 + 2.10\cdot10^{2}\cdot F_{in,EC12}^2 - 1.23\cdot10^{-2}\cdot\left(\frac{F_{in,EC0}}{F_{in,EC12}}\right)^2 - 9.19\cdot10^{-5}\cdot V_{sl}^2 - 1.08\cdot10^{-9}\cdot\left(\frac{V_{sl}}{F_{in,EC12}}\right)^2$$
$$- 6.11\cdot10^{-11}\cdot(V_{sl}\cdot C_{sl})^2 - 4.55\cdot10^{-6}\cdot T\cdot C_{sl} + 4.46\cdot10^{-2}\cdot T\cdot F_{in,EC12} - 8.67\cdot10^{-4}\cdot T\cdot\frac{F_{in,EC0}}{F_{in,EC12}} - 3.39\cdot10^{-5}\cdot T\cdot V_{sl}$$
$$+ 8.71\cdot10^{-2}\cdot T\cdot F_{in,EC8} + 2.02\cdot10^{-2}\cdot T\cdot F_{in,EC4} - 2.86\cdot10^{-8}\cdot T\cdot\frac{V_{sl}}{F_{in,EC12}} + 2.24\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC12}$$
$$- 2.03\cdot10^{-4}\cdot C_{sl}\cdot\frac{F_{in,EC0}}{F_{in,EC12}} + 1.61\cdot10^{-2}\cdot C_{sl}\cdot F_{in,EC8} + 1.18\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC4} - 7.85\cdot10^{-8}\cdot C_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}}$$
$$+ 1.47\cdot10^{-8}\cdot V_{sl}\cdot C_{sl}^2 + 2.17\cdot F_{in,EC0} + 6.45\cdot10^{-2}\cdot F_{in,EC12}\cdot V_{sl} + 1.15\cdot10^{2}\cdot F_{in,EC12}\cdot F_{in,EC8}$$
$$+ 4.33\cdot10^{1}\cdot F_{in,EC12}\cdot F_{in,EC4} + 6.47\cdot10^{-5}\cdot F_{in,EC12}\cdot V_{sl}\cdot C_{sl} - 2.13\cdot10^{-3}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl} - 4.29\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot F_{in,EC4}$$
$$+ 6.14\cdot10^{-6}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot\frac{V_{sl}}{F_{in,EC12}} + 2.40\cdot10^{-6}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl} + 8.36\cdot10^{-2}\cdot V_{sl}\cdot F_{in,EC8} + 1.96\cdot10^{-7}\cdot V_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}}$$
$$+ 1.60\cdot10^{-8}\cdot V_{sl}^2\cdot C_{sl} + 3.41\cdot10^{-4}\cdot F_{in,EC8}\cdot\frac{V_{sl}}{F_{in,EC12}} - 1.46\cdot10^{-4}\cdot F_{in,EC8}\cdot V_{sl}\cdot C_{sl} + 1.11\cdot10^{-4}\cdot F_{in,EC4}\cdot\frac{V_{sl}}{F_{in,EC12}}$$
$$+ 9.08\cdot10^{-10}\cdot\frac{V_{sl}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl} \tag{S48}$$

$$\frac{F_{out,EC4}}{F_{in,EC12}+F_{in,EC8}+F_{in,EC4}} = 1.58\cdot10^{-3}\cdot T - 3.97\cdot10^{-4}\cdot C_{sl} - 1.57\cdot F_{in,EC12} + 4.74\cdot10^{-2}\cdot\frac{F_{in,EC0}}{F_{in,EC12}} + 1.05\cdot10^{-3}\cdot V_{sl}$$
$$+ 1.88\cdot10^{1}\cdot F_{in,EC8} + 4.58\cdot10^{1}\cdot F_{in,EC4} - 5.15\cdot10^{-5}\cdot\frac{V_{sl}}{F_{in,EC12}} - 1.33\cdot10^{-5}\cdot V_{sl}\cdot C_{sl} - 2.89\cdot10^{-6}\cdot T^2 + 1.36\cdot10^{-7}\cdot C_{sl}^2$$
$$- 7.21\cdot10^{1}\cdot F_{in,EC12}^2 - 2.31\cdot10^{-3}\cdot\left(\frac{F_{in,EC0}}{F_{in,EC12}}\right)^2 - 1.90\cdot10^{-5}\cdot V_{sl}^2 - 8.69\cdot10^{-10}\cdot\left(\frac{V_{sl}}{F_{in,EC12}}\right)^2 - 3.46\cdot10^{-11}\cdot(V_{sl}\cdot C_{sl})^2$$
$$+ 2.54\cdot10^{-7}\cdot T\cdot C_{sl} + 9.80\cdot10^{-3}\cdot T\cdot F_{in,EC12} - 6.69\cdot10^{-5}\cdot T\cdot\frac{F_{in,EC0}}{F_{in,EC12}} - 7.06\cdot10^{-6}\cdot T\cdot V_{sl} - 2.99\cdot10^{-2}\cdot T\cdot F_{in,EC8}$$
$$- 7.66\cdot10^{-2}\cdot T\cdot F_{in,EC4} + 9.09\cdot10^{-8}\cdot T\cdot\frac{V_{sl}}{F_{in,EC12}} + 1.85\cdot10^{-8}\cdot T\cdot V_{sl}\cdot C_{sl} + 5.35\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC12}$$
$$+ 1.05\cdot10^{-5}\cdot C_{sl}\cdot\frac{F_{in,EC0}}{F_{in,EC12}} - 4.39\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC8} - 1.50\cdot10^{-2}\cdot C_{sl}\cdot F_{in,EC4} + 4.52\cdot10^{-8}\cdot C_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}}$$
$$+ 3.25\cdot10^{-9}\cdot V_{sl}\cdot C_{sl}^2 - 1.69\cdot10^{-1}\cdot F_{in,EC0} + 6.99\cdot10^{-2}\cdot F_{in,EC12}\cdot V_{sl} - 3.32\cdot10^{1}\cdot F_{in,EC12}\cdot F_{in,EC8}$$
$$- 1.02\cdot10^{1}\cdot F_{in,EC12}\cdot F_{in,EC4} - 9.80\cdot10^{-5}\cdot F_{in,EC12}\cdot V_{sl}\cdot C_{sl} + 2.16\cdot10^{-4}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl} - 1.13\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot F_{in,EC8}$$
$$+ 4.81\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot F_{in,EC4} - 1.37\cdot10^{-6}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot\frac{V_{sl}}{F_{in,EC12}} - 3.73\cdot10^{-7}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl} - 2.30\cdot10^{-2}\cdot V_{sl}\cdot F_{in,EC8}$$
$$- 1.03\cdot10^{-1}\cdot V_{sl}\cdot F_{in,EC4} + 4.10\cdot10^{-7}\cdot V_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}} + 8.01\cdot10^{-8}\cdot V_{sl}^2\cdot C_{sl} - 5.05\cdot10^{1}\cdot F_{in,EC8}\cdot F_{in,EC4}$$
$$- 9.52\cdot10^{-5}\cdot F_{in,EC8}\cdot\frac{V_{sl}}{F_{in,EC12}} + 3.33\cdot10^{-5}\cdot F_{in,EC8}\cdot V_{sl}\cdot C_{sl} - 3.45\cdot10^{-5}\cdot F_{in,EC4}\cdot\frac{V_{sl}}{F_{in,EC12}} + 1.78\cdot10^{-4}\cdot F_{in,EC4}\cdot V_{sl}\cdot C_{sl}$$
$$- 5.32\cdot10^{-10}\cdot\frac{V_{sl}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl} \tag{S49}$$

$$
\begin{aligned}
\frac{F_{out,EC8}}{F_{in,EC12}+F_{in,EC8}} &= 2.47\cdot10^{-3}\cdot T - 6.14\cdot10^{-4}\cdot C_{sl} + 4.99\cdot F_{in,EC12} + 7.75\cdot10^{-2}\cdot\frac{F_{in,EC0}}{F_{in,EC12}} + 3.61\cdot10^{-4}\cdot V_{sl}\\
&+ 5.22\cdot10^{1}\cdot F_{in,EC8} + 1.98\cdot10^{1}\cdot F_{in,EC4} - 7.23\cdot10^{-5}\cdot\frac{V_{sl}}{F_{in,EC12}} - 2.41\cdot10^{-5}\cdot V_{sl}\cdot C_{sl} - 4.37\cdot10^{-6}\cdot T^2 + 3.73\cdot10^{-7}\cdot C_{sl}^2\\
&- 1.41\cdot10^{2}\cdot F_{in,EC12}^2 - 4.95\cdot10^{-3}\cdot\left(\frac{F_{in,EC0}}{F_{in,EC12}}\right)^2 - 1.28\cdot10^{-5}\cdot V_{sl}^2 - 9.24\cdot10^{-10}\cdot\left(\frac{V_{sl}}{F_{in,EC12}}\right)^2 - 6.56\cdot10^{-11}\cdot(V_{sl}\cdot C_{sl})^2\\
&+ 7.21\cdot10^{-3}\cdot T\cdot F_{in,EC12} - 9.24\cdot10^{-5}\cdot T\cdot\frac{F_{in,EC0}}{F_{in,EC12}} - 1.12\cdot10^{-5}\cdot T\cdot V_{sl} - 8.19\cdot10^{-2}\cdot T\cdot F_{in,EC8} - 2.76\cdot10^{-2}\cdot T\cdot F_{in,EC4}\\
&+ 1.23\cdot10^{-7}\cdot T\cdot\frac{V_{sl}}{F_{in,EC12}} + 3.73\cdot10^{-8}\cdot T\cdot V_{sl}\cdot C_{sl} + 7.12\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC12} + 1.59\cdot10^{-5}\cdot C_{sl}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\\
&- 1.87\cdot10^{-2}\cdot C_{sl}\cdot F_{in,EC8} - 4.56\cdot10^{-3}\cdot C_{sl}\cdot F_{in,EC4} + 8.48\cdot10^{-8}\cdot C_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}} + 4.97\cdot10^{-9}\cdot V_{sl}\cdot C_{sl}^2\\
&- 5.18\cdot10^{-2}\cdot F_{in,EC0} + 8.13\cdot10^{-2}\cdot F_{in,EC12}\cdot V_{sl} - 5.10\cdot10^{1}\cdot F_{in,EC12}\cdot F_{in,EC8} - 7.33\cdot10^{1}\cdot F_{in,EC12}\cdot F_{in,EC4}\\
&- 1.56\cdot10^{-4}\cdot F_{in,EC12}\cdot V_{sl}\cdot C_{sl} + 3.03\cdot10^{-4}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl} + 2.69\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot F_{in,EC8} - 4.93\cdot10^{-1}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot F_{in,EC4}\\
&- 2.01\cdot10^{-6}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot\frac{V_{sl}}{F_{in,EC12}} - 7.76\cdot10^{-7}\cdot\frac{F_{in,EC0}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl} - 1.19\cdot10^{-1}\cdot V_{sl}\cdot F_{in,EC8} - 1.38\cdot10^{-2}\cdot V_{sl}\cdot F_{in,EC4}\\
&+ 5.31\cdot10^{-7}\cdot V_{sl}\cdot\frac{V_{sl}}{F_{in,EC12}} + 1.40\cdot10^{-7}\cdot V_{sl}^2\cdot C_{sl} + 7.40\cdot F_{in,EC8}\cdot F_{in,EC4} - 1.57\cdot10^{-4}\cdot F_{in,EC8}\cdot\frac{V_{sl}}{F_{in,EC12}}\\
&+ 2.09\cdot10^{-4}\cdot F_{in,EC8}\cdot V_{sl}\cdot C_{sl} - 2.07\cdot10^{-4}\cdot F_{in,EC4}\cdot\frac{V_{sl}}{F_{in,EC12}} + 1.77\cdot10^{-5}\cdot F_{in,EC4}\cdot V_{sl}\cdot C_{sl} - 1.00\cdot10^{-9}\cdot\frac{V_{sl}}{F_{in,EC12}}\cdot V_{sl}\cdot C_{sl}
\end{aligned}
\tag{S50}
$$

2.8.2 Trickle bed reactors

The trickle bed dehydrogenation yields for NEC system compounds are included in Equations (S51-S53).

$$\frac{F_{out,EC0}}{F_{in,EC12}+F_{in,EC8}+F_{in,EC4}+F_{in,EC0}} = 3.53\cdot10^{-3}\cdot T_{in} + 2.34\cdot10^{-2}\cdot D + 1.62\cdot10^{-3}\cdot L_{in} - 3.08\cdot10^{-6}\cdot W_{cat}$$
$$+ 7.45\cdot F_{in,EC0} - 8.55\cdot10^{1}\cdot F_{in,EC12} - 2.25\cdot10^{2}\cdot F_{in,EC8} - 5.96\cdot10^{1}\cdot F_{in,EC4} - 1.36\cdot10^{-8}\cdot\frac{W_{cat}}{F_{in,EC12}}$$
$$- 3.43\cdot10^{-6}\cdot T_{in}^2 - 4.02\cdot10^{-4}\cdot L_{in}^2 - 1.58\cdot F_{in,EC0}^2 - 1.11\cdot10^{3}\cdot F_{in,EC12}^2 - 1.42\cdot10^{4}\cdot F_{in,EC8}^2$$
$$- 1.00\cdot10^{-16}\cdot\left(\frac{W_{cat}}{F_{in,EC12}}\right)^2 - 4.88\cdot10^{-5}\cdot T_{in}\cdot D + 1.08\cdot10^{-8}\cdot T_{in}\cdot W_{cat} - 2.36\cdot10^{-3}\cdot T_{in}\cdot F_{in,EC0}$$
$$+ 1.97\cdot10^{-2}\cdot T_{in}\cdot F_{in,EC12} + 5.27\cdot10^{-2}\cdot T_{in}\cdot F_{in,EC8} + 3.05\cdot10^{-2}\cdot T_{in}\cdot F_{in,EC4} + 3.98\cdot10^{-11}\cdot T_{in}\cdot\frac{W_{cat}}{F_{in,EC12}}$$
$$+ 3.87\cdot10^{-3}\cdot D\cdot L_{in} + 7.64\cdot10^{-3}\cdot D\cdot G_{in} - 3.35\cdot10^{-7}\cdot D\cdot W_{cat} - 1.66\cdot D\cdot F_{in,EC0} + 1.92\cdot10^{1}\cdot D\cdot F_{in,EC12}$$
$$+ 5.61\cdot10^{1}\cdot D\cdot F_{in,EC8} + 1.15\cdot10^{1}\cdot D\cdot F_{in,EC4} - 2.72\cdot10^{-10}\cdot D\cdot\frac{W_{cat}}{F_{in,EC12}} - 3.18\cdot10^{-3}\cdot L_{in}\cdot G_{in}$$
$$- 1.25\cdot10^{-7}\cdot L_{in}\cdot W_{cat} - 5.10\cdot10^{-1}\cdot L_{in}\cdot F_{in,EC0} + 5.28\cdot L_{in}\cdot F_{in,EC12} + 1.92\cdot10^{1}\cdot L_{in}\cdot F_{in,EC8}$$
$$+ 3.24\cdot L_{in}\cdot F_{in,EC4} + 6.00\cdot10^{-10}\cdot L_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 4.39\cdot10^{-1}\cdot G_{in}\cdot F_{in,EC0} + 3.82\cdot G_{in}\cdot F_{in,EC12}$$
$$+ 1.16\cdot10^{-8}\cdot G_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 1.44\cdot10^{-6}\cdot W_{cat}\cdot F_{in,EC0} + 2.83\cdot10^{-5}\cdot W_{cat}\cdot F_{in,EC12} + 4.37\cdot10^{-5}\cdot W_{cat}\cdot F_{in,EC4}$$
$$- 5.60\cdot10^{-15}\cdot W_{cat}\cdot\frac{W_{cat}}{F_{in,EC12}} + 1.34\cdot10^{2}\cdot F_{in,EC0}\cdot F_{in,EC12} + 4.50\cdot10^{2}\cdot F_{in,EC0}\cdot F_{in,EC8}$$
$$+ 1.75\cdot10^{1}\cdot F_{in,EC0}\cdot F_{in,EC4} - 5.87\cdot10^{-8}\cdot F_{in,EC0}\cdot\frac{W_{cat}}{F_{in,EC12}} - 9.41\cdot10^{3}\cdot F_{in,EC12}\cdot F_{in,EC8}$$
$$- 7.59\cdot10^{2}\cdot F_{in,EC12}\cdot F_{in,EC4} - 3.15\cdot10^{3}\cdot F_{in,EC8}\cdot F_{in,EC4} + 1.26\cdot10^{-6}\cdot F_{in,EC8}\cdot\frac{W_{cat}}{F_{in,EC12}}$$
$$+ 5.85\cdot10^{-7}\cdot F_{in,EC4}\cdot\frac{W_{cat}}{F_{in,EC12}} \tag{S51}$$

$$\frac{F_{out,EC4}}{F_{in,EC12}+F_{in,EC8}+F_{in,EC4}} = -8.27\cdot10^{-4}\cdot T_{in} + 3.49\cdot10^{-2}\cdot L_{in} + 1.38\cdot G_{in} - 6.61\cdot10^{-6}\cdot W_{cat} - 3.74\cdot F_{in,EC0}$$
$$+ 2.36\cdot10^{2}\cdot F_{in,EC8} + 5.50\cdot10^{2}\cdot F_{in,EC4} + 1.53\cdot10^{-7}\cdot\frac{W_{cat}}{F_{in,EC12}} + 2.25\cdot10^{-6}\cdot T_{in}^2 - 2.83\cdot10^{-3}\cdot D^2$$
$$+ 1.01\cdot10^{-3}\cdot L_{in}^2 - 8.37\cdot10^{-11}\cdot W_{cat}^2 + 2.39\cdot10^{-1}\cdot F_{in,EC0}^2 + 1.30\cdot10^{4}\cdot F_{in,EC8}^2 - 9.51\cdot10^{2}\cdot F_{in,EC4}^2$$
$$- 8.00\cdot10^{-16}\cdot\left(\frac{W_{cat}}{F_{in,EC12}}\right)^2 - 9.05\cdot10^{-5}\cdot T_{in}\cdot L_{in} - 2.39\cdot10^{-3}\cdot T_{in}\cdot G_{in} + 6.21\cdot10^{-9}\cdot T_{in}\cdot W_{cat} + 2.18\cdot10^{-3}\cdot T_{in}\cdot F_{in,EC0}$$
$$- 3.84\cdot10^{-1}\cdot T_{in}\cdot F_{in,EC4} - 2.90\cdot10^{-10}\cdot T_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 6.95\cdot10^{-3}\cdot D\cdot L_{in} + 2.20\cdot10^{-6}\cdot D\cdot W_{cat} + 7.16\cdot10^{-1}\cdot D\cdot F_{in,EC0}$$
$$- 6.07\cdot10^{1}\cdot D\cdot F_{in,EC8} - 8.75\cdot10^{1}\cdot D\cdot F_{in,EC4} + 8.31\cdot10^{-10}\cdot D\cdot\frac{W_{cat}}{F_{in,EC12}} - 4.91\cdot10^{-2}\cdot L_{in}\cdot G_{in} + 7.82\cdot10^{-7}\cdot L_{in}\cdot W_{cat}$$
$$+ 2.11\cdot10^{-1}\cdot L_{in}\cdot F_{in,EC0} + 4.11\cdot10^{-1}\cdot L_{in}\cdot F_{in,EC12} - 2.30\cdot10^{1}\cdot L_{in}\cdot F_{in,EC8} - 2.35\cdot10^{1}\cdot L_{in}\cdot F_{in,EC4}$$
$$+ 5.32\cdot10^{-9}\cdot L_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 7.87\cdot10^{-1}\cdot G_{in}\cdot F_{in,EC0} + 5.10\cdot10^{1}\cdot G_{in}\cdot F_{in,EC8} + 4.53\cdot10^{1}\cdot G_{in}\cdot F_{in,EC4}$$
$$- 5.83\cdot10^{-8}\cdot G_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 1.51\cdot10^{-5}\cdot W_{cat}\cdot F_{in,EC0} + 1.09\cdot10^{-4}\cdot W_{cat}\cdot F_{in,EC12} - 6.41\cdot10^{-4}\cdot W_{cat}\cdot F_{in,EC8}$$
$$- 2.75\cdot10^{-4}\cdot W_{cat}\cdot F_{in,EC4} - 4.17\cdot10^{1}\cdot F_{in,EC0}\cdot F_{in,EC12} - 1.65\cdot10^{2}\cdot F_{in,EC0}\cdot F_{in,EC8} + 7.07\cdot10^{1}\cdot F_{in,EC0}\cdot F_{in,EC4}$$
$$+ 1.13\cdot10^{-7}\cdot F_{in,EC0}\cdot\frac{W_{cat}}{F_{in,EC12}} + 5.88\cdot10^{3}\cdot F_{in,EC12}\cdot F_{in,EC8} + 2.41\cdot10^{3}\cdot F_{in,EC12}\cdot F_{in,EC4} + 1.58\cdot10^{4}\cdot F_{in,EC8}\cdot F_{in,EC4}$$
$$- 4.31\cdot10^{-6}\cdot F_{in,EC8}\cdot\frac{W_{cat}}{F_{in,EC12}} - 1.38\cdot10^{-5}\cdot F_{in,EC4}\cdot\frac{W_{cat}}{F_{in,EC12}} \tag{S52}$$

$$\frac{F_{out,EC8}}{F_{in,EC12}+F_{in,EC8}} = 9.13\cdot10^{-4}\cdot T_{in} - 1.45\cdot10^{-1}\cdot D - 3.15\cdot10^{-2}\cdot L_{in} + 3.93\cdot10^{-1}\cdot G_{in} - 4.89\cdot F_{in,EC0} - 3.03\cdot10^{1}\cdot F_{in,EC12}$$
$$+ 9.34\cdot10^{2}\cdot F_{in,EC8} - 2.93\cdot F_{in,EC4} + 1.39\cdot10^{-7}\cdot\frac{W_{cat}}{F_{in,EC12}} - 4.68\cdot10^{-7}\cdot T_{in}^2 - 1.44\cdot10^{-2}\cdot D^2 + 3.33\cdot10^{-3}\cdot L_{in}^2 - 2.23\cdot G_{in}^2$$
$$- 3.53\cdot10^{-10}\cdot W_{cat}^2 + 2.56\cdot10^{-1}\cdot F_{in,EC0}^2 - 1.66\cdot10^{3}\cdot F_{in,EC12}^2 + 5.64\cdot10^{4}\cdot F_{in,EC8}^2 - 3.00\cdot10^{-16}\cdot\left(\frac{W_{cat}}{F_{in,EC12}}\right)^2$$
$$+ 3.87\cdot10^{-4}\cdot T_{in}\cdot D - 8.08\cdot10^{-8}\cdot T_{in}\cdot W_{cat} + 5.15\cdot10^{-3}\cdot T_{in}\cdot F_{in,EC0} - 5.50\cdot10^{-1}\cdot T_{in}\cdot F_{in,EC8} - 3.10\cdot10^{-10}\cdot T_{in}\cdot\frac{W_{cat}}{F_{in,EC12}}$$
$$- 1.04\cdot10^{-2}\cdot D\cdot L_{in} + 4.71\cdot10^{-6}\cdot D\cdot W_{cat} + 5.26\cdot10^{-1}\cdot D\cdot F_{in,EC0} + 1.16\cdot10^{1}\cdot D\cdot F_{in,EC12} - 1.69\cdot10^{2}\cdot D\cdot F_{in,EC8}$$
$$- 4.53\cdot10^{-9}\cdot D\cdot\frac{W_{cat}}{F_{in,EC12}} - 9.03\cdot10^{-2}\cdot L_{in}\cdot G_{in} + 2.18\cdot10^{-6}\cdot L_{in}\cdot W_{cat} + 8.14\cdot10^{-2}\cdot L_{in}\cdot F_{in,EC0} + 5.34\cdot L_{in}\cdot F_{in,EC12}$$
$$- 6.38\cdot10^{1}\cdot L_{in}\cdot F_{in,EC8} + 6.09\cdot10^{-9}\cdot L_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 5.54\cdot10^{-6}\cdot G_{in}\cdot W_{cat} - 3.51\cdot G_{in}\cdot F_{in,EC0} + 4.06\cdot10^{1}\cdot G_{in}\cdot F_{in,EC12}$$
$$+ 1.58\cdot10^{2}\cdot G_{in}\cdot F_{in,EC8} - 5.44\cdot10^{-8}\cdot G_{in}\cdot\frac{W_{cat}}{F_{in,EC12}} - 1.46\cdot10^{-5}\cdot W_{cat}\cdot F_{in,EC0} + 1.93\cdot10^{-4}\cdot W_{cat}\cdot F_{in,EC12}$$
$$- 1.67\cdot10^{-3}\cdot W_{cat}\cdot F_{in,EC8} - 1.48\cdot10^{-4}\cdot W_{cat}\cdot F_{in,EC4} + 6.16\cdot10^{-13}\cdot W_{cat}\cdot\frac{W_{cat}}{F_{in,EC12}} + 9.89\cdot10^{1}\cdot F_{in,EC0}\cdot F_{in,EC8}$$
$$+ 3.06\cdot10^{-7}\cdot F_{in,EC0}\cdot\frac{W_{cat}}{F_{in,EC12}} + 2.20\cdot10^{3}\cdot F_{in,EC12}\cdot F_{in,EC8} + 3.07\cdot10^{-5}\cdot W_{cat} + 1.98\cdot10^{3}\cdot F_{in,EC8}\cdot F_{in,EC4}$$
$$- 1.99\cdot10^{-5}\cdot F_{in,EC8}\cdot\frac{W_{cat}}{F_{in,EC12}} + 2.14\cdot10^{-6}\cdot F_{in,EC4}\cdot\frac{W_{cat}}{F_{in,EC12}} \tag{S53}$$

2.9 Equipment costs estimation

To estimate the cost of the process equipment, different correlations are taken from literature. The cost of heat exchangers and pumps is obtained from Sinnott and Towler (2020d) based on the heat exchange area and the volumetric flow respectively. The purchase cost of the compressors is based on the correlation from Couper et al. (2005). The vessels wall thickness is estimated based on Sinnott and Towler (2020c). Then, the weight of the reactor and flash vessels is calculated. This allows to estimate the cost of these vessels from Sinnott and Towler (2020d). In the case of the reactors, for both trickle and slurry reactors, the cost of the catalyst is also included (500\$/kg$_{cat}$) (Dutta et al., 2016). Furthermore, for the slurry reactor design, the cost of the heat exchange devices is estimated as a shell and tube heat exchanger from Sinnott and Towler (2020d).

3 Hydrogenation and dehydrogenation investment costs

Additionally, Figure S1 is included showing the investment costs for hydrogenation, dehydrogenation processes and the sum of both.

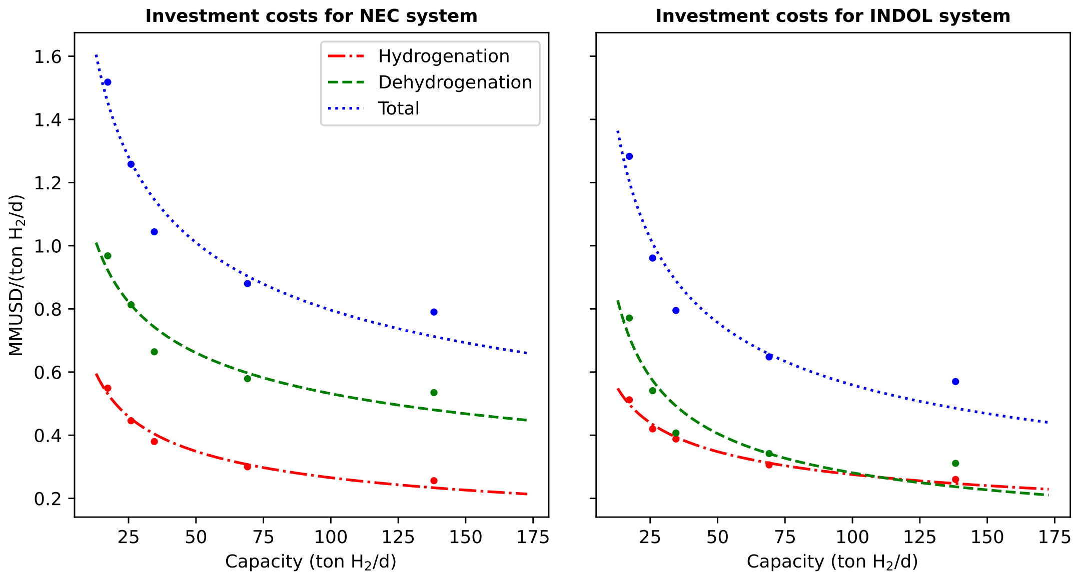

Figure S1: Investment costs for NEC and INDOL systems against plant capacity

4 Nomenclature

A	Heat transfer area (m^2)
D	Reactor diameter (m)
Cp	Specific heat (kJ/kg· K)
C_{sl}	Catalyst concentration in the slurry phase (kg/m^3)
F	Molar flow (kmol/s)
F&EI	Fire and Explosion Index
G_{in}	Gas flowrate ($kg/m^2 \cdot s$)
H	Stream enthalpy (kW)
He	Henry coefficient (bar)
ΔHr	Reaction enthalpy (kJ/kmol)
k	Politropic constant
L_{in}	Liquid flowrate ($kg/m^2 \cdot s$)
n_{cp}	Number of compressors
P	Pressure (bar)
Pen	F&EI Penalty
P_v	Vapor pressure (bar)
Q	Heat demand (kW)
R	Ideal gas constant (J/mol· K)
r_p	Compression ratio

T	Temperature (K)
ΔT_{log}	Logarithmic temperature difference (K)
U	Overall heat transfer coefficient (kW/$m^2\cdot$ K)
$u_{g,0}$	Superficial gas velocity (m/s)
$\dot{V}$	Volumetric flow (m^3/s)
V_{sl}	Slurry volume (m^3)
W	Power (kW)
W_{cat}	Catalyst weight (kg)
X	Conversion
x	Stream composition
c	Stream component index
i	Inlet streams index
j	Outlet streams index
η	Yield
λ	Latent heat (kJ/kg)
μ_{JT}	Joule-Thomson coefficient (K/bar)

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