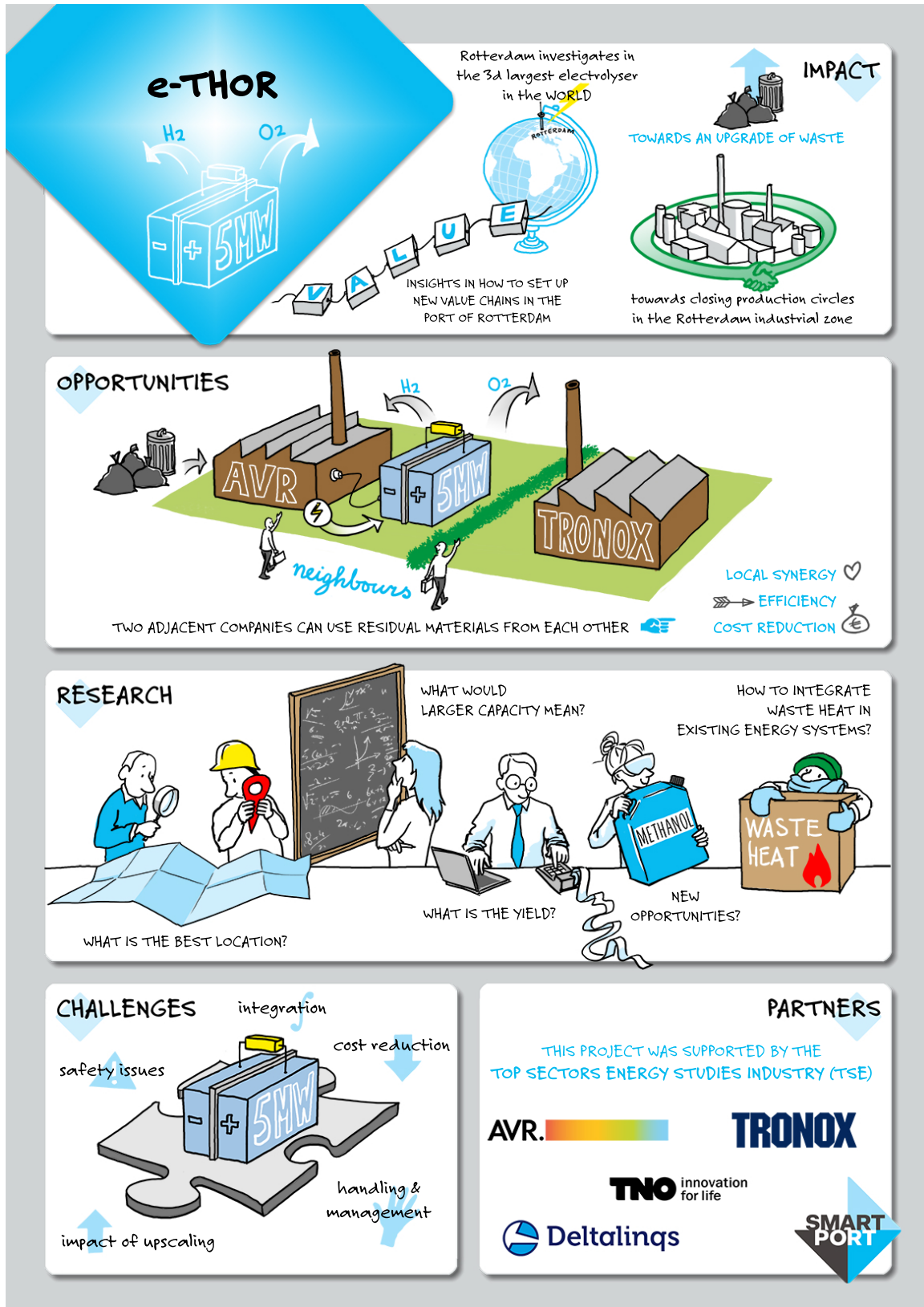


Electrolysis Technology for Hydrogen and Oxygen production in Rotterdam ("e-THOR")



Publiek Eindrapport

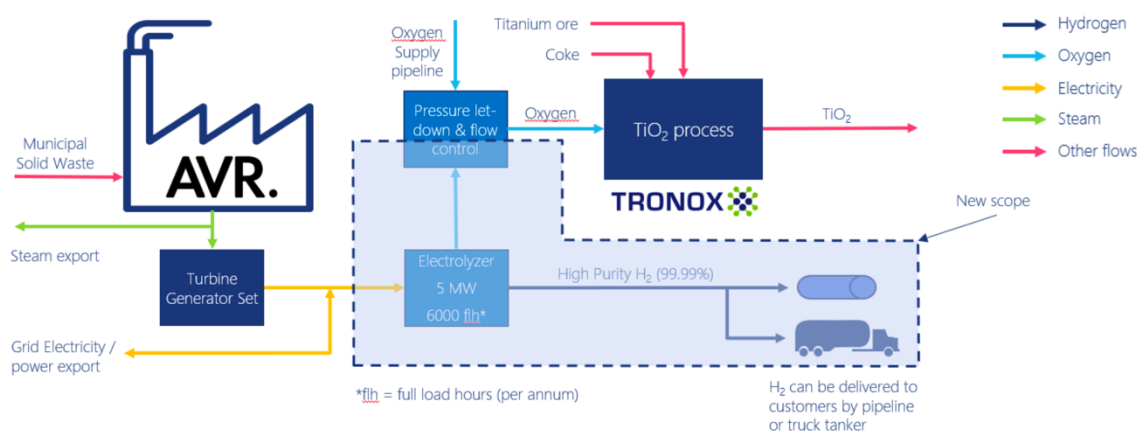
Electrolysis Technology for Hydrogen and Oxygen production in Rotterdam ("e-THOR"), (ref RVO:TESN119011)

1. Summary and introduction

The e-THOR concept(s) integrate the production and use of Hydrogen (H_2), Oxygen (O_2) and low temperature heat in the local energy value chain in Rotterdam. Being a waste incinerator, AVR serves an essential purpose for significant non-fossil electricity production and as a key and robust partner in energy value chain. There is an opportunity to utilize the electricity generated by AVR to feed an electrolyzer. The products such as H_2 , waste heat and O_2 from electrolysis can be all used locally for supporting significant reduction of CO_2 . Furthermore, the O_2 might be used to increase the circularity of carbon by its conversion to methanol which can be further be used in production of chemicals (e.g. polymers) by other companies in the value chain.

AVR and Tronox are two companies that due to their proximity may allow for synergies: AVR avails of in-house produced electricity that could be converted to hydrogen and oxygen, whereas Tronox uses oxygen in its core process and has some of carbon monoxide (CO) as by-product. In order to quantify the opportunity, in the period 01-Oct-2019 - 01-May-2020, a consortium of AVR, Tronox, TNO and Deltalinqs have carried out - with financial support from Topsector Energiesubsidie van het Ministerie van Economische Zaken - a joint initial investigation into the viability of a 5 MW water-electrolyzer to produce hydrogen (H_2), oxygen (O_2) and heat. If deemed attractive enough, the installation is envisaged to be located at AVR, with the aim to eventually extend this into a 100 MW electrolyzer.

The concept - whereby also the byproducts heat and oxygen are to be utilized - is shown in the picture below.



The study has evaluated - technically and economically - a number of routes to make use of the synergy opportunity between these companies with as guiding aim the reduction of CO_2 emissions:

- 1) Electrolysis of water to produce hydrogen, heat and oxygen both at ~5 MW scale and ~100 MW scale.
- 2) Applying the TNO SEWGS© technology to produce hydrogen from Tronox' CO-rich byproducts
- 3) Utilizing AVR's potential hydrogen to convert Tronox' CO into methanol.

In order to better understand the feasibility and robustness of such electrolyzer facility typically the following elements have to be addressed (TECOP):

(T)echnology robustness – does it work?

(E)conomics – how expensive versus alternatives?

(C)ontractual elements/supply chain partners – can it be implemented?

(O)rganisational capabilities – can it be built and operated?

(P)olitical – is it acceptable?

To address a part of the above aspects to help establish feasibility, the study looked into technology and high-level economics:

- Inventory of possible implementation options at AVR (T)
- Modeling of the 5 MW demo system and extrapolation to a 100 MW future plant (T)
- CAPEX estimate for the 5 MW system and forecast for a 100 MW version (T, E)
- Quantification of plant output: H₂-flow, O₂-flow and waste heat for the selected operating conditions (T, E)
- Conduction of a sensitivity analysis to assess the impact of CAPEX, utilization and power price on the H₂ production cost (E)
- Potential H₂ outlets to identify economical feasibility of this concept (E)
- Evaluation at high-level of some alternative routes for decarbonization of Tronox (T,E)

From the investigation a number of preliminary conclusions have been drawn.

For hydrogen production, both at 5 MW and 100 MW scale the bare production cost of hydrogen would – despite some potential cost benefits contingent upon selling O₂ to Tronox and/or an industrial gas supplier and using the waste heat at AVR - be significantly higher than current hydrogen prices. Economy of scale would make 100 MW some 20% cheaper than 5 MW, yet it became clear that the predominant cost factor in both cases would be the price of electricity. The best way of monetizing this AVR hydrogen would be found in special niches or in the mobility sector, where hydrogen commands much higher prices than in industrial use.

Another way to benefit from proximity of the two companies and linked to the AVR hydrogen ambitions, would be presented by converting Tronox waste CO into additional H₂. Such process could make use of the TNO SEWGS® technology and thus yield hydrogen by converting CO. A byproduct of this process is 95% pure pressurized CO₂ which is CCS capture-ready without requiring large capturing equipment. Also the sales of the produced (blue) hydrogen would contribute significantly to a lower cost. If this process is compared to the main alternative decarbonization pathway for Tronox - amine treating of the CO₂-rich waste gas after incineration – it would compare favorably at an overall abatement cost. Note that the presence of N₂ in the gas depresses economic viability, hence removal of N₂ from the stream would help the CO₂ abatement cost further. This, however, has not been quantified further in this study

The final option that has been evaluated was production of methanol from Tronox CO-rich gas and hydrogen supplied by AVR. The resulting syngas would be converted to methanol with available technology. The economic evaluation showed that produced in this way and at the scale feasible at Tronox, the methanol would cost almost double that of the current methanol market price. Hence this would currently not be economically viable, unless like with hydrogen, special niches could be found. Also in this case, removal of nitrogen from the waste gas stream would likely improve the economics, yet has not been quantified further in this study.

The estimated CO₂ benefits from these evaluated pathways depend strongly on alternatives for the electricity and do require a more detailed Life-Cycle-Analysis (LCA). However, as a first indication and based on premises such as availability of green electricity as alternative, CO₂ reductions could range anywhere between 1.5 kta to 130 kta. This wide range illustrates the existing uncertainties because it includes the demo case. Please refer to section 3 for further discussions.

Following the results of this study AVR and Tronox have first of all obtained a much better understanding of the business case mechanisms such as the advantage of an integrated approach, the benefits of byproducts Oxygen and low temperature waste heat and the impact of scale. AVR has recently started the activity to look deeper into the markets for green hydrogen and ways to finance an engineering and/or a construction phase. Finally, contact will be made with a company that has a business in Methanol to assess whether the Methanol synthesis of CO from Tronox, with green hydrogen would be a feasible route.

At current market-conditions the above opportunities could only come to fruition if simultaneously a number of requirements could be met:

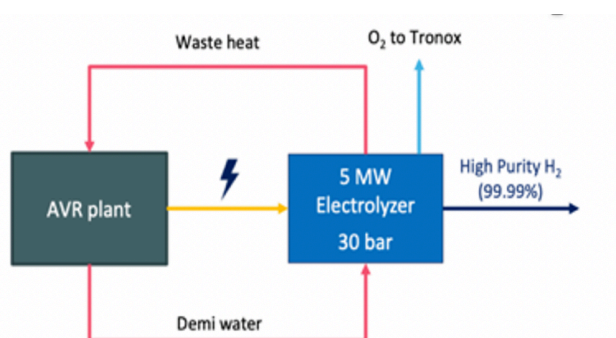
- Have off-take agreements with H₂ users to ensure that (partially) green H₂ can be sold at a price above the gray H₂ market to fulfill certain “green” market needs.
- Ensure that the void left by AVR when directing their electricity away from the grid is fulfilled by green sources or not required at all (easier for small scale electrolysis)
- Reduce the CAPEX component of the overall production costs through green H₂ subsidy support (e.g. DEI+ or SDE++)
- Ensure proper electrolyzer integration for additional revenue; i.e. agreement with Tronox or industrial gas suppliers to sell co-produced O₂ and waste heat utilization
- Evaluate in more detail the possibility of signing a grid services contract with TenneT to lower the overall cost of electricity.
- Make use of low electricity prices through flexible operation of the electrolyzer.
- For the methanol case, the most important aspect is finding an interested off-taker for the (partially) green methanol - with its cost being well above market price. The potential upside of CAPEX subsidies is much smaller in this case, because the production costs are dominated by OPEX (H₂).
- Note that for Tronox, the use of SEWGS® technology would already pose a solid alternative to conventional CO₂ capture technologies. Reduction of nitrogen content in the feed-gas from Tronox would be worth investigating.
- Both H₂ and methanol production in the concepts evaluated in this study would benefit from adequate certification. For H₂, the approach defined under the CertifHY project is recommended and it is expected that the H₂ produced by the 5 MW demo could be certified as (at least partially) green.

2. Brief discussion of the studied elements

2.1 Investigate a 5 MW Electrolyzer to produce merchant hydrogen

In agreement with AVR and Tronox it was decided to initially aim in this case-study for a 4.7 MW alkaline electrolyzer, operating to deliver hydrogen at elevated pressure, as this would be large enough to be potentially commercially viable, yet small enough to allow for affordable risk in CAPEX expenditure in case of favorable outcomes. Furthermore, alkaline technology was selected over PEM technology for reasons of cost and commercial experience (reliability). This is, however, a preliminary technology choice for the feasibility study, and the final technology selection would be done in the basic design phase of the pilot project. This scale of unit is at the moment significant enough to be interesting when compared to other electrolyzer projects in the industry.

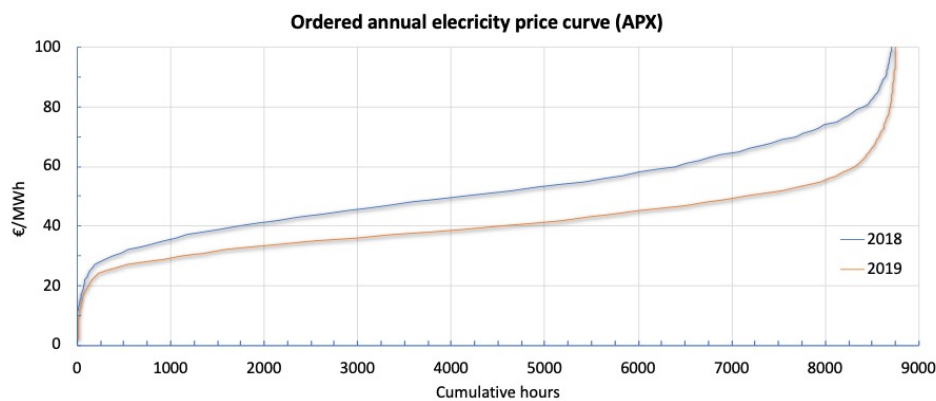
After discussions with Tronox and AVR, the investigated constellation along with some important parameters obtained by TNO from electrolyzer suppliers was as shown in the picture below. The byproducts of a water-electrolyzer, heat and oxygen, will be utilized by AVR resp. Tronox. Some of the most important premises will be discussed in more detail below.



As shown in the picture below, the envisaged AVR plant would supply 4.7 MWe of in-house generated electricity to an alkaline-type electrolyzer. During the process of electrolysis some of the power is converted to waste heat (a typical operating temperature is 80 °C). It is estimated that this unit would conservatively produce 1 standard m³ of hydrogen for each 4.7 kWh of electrical energy input or an overall electric efficiency (in case hydrogen would be used for combustion) of almost 64%. As each m³ of hydrogen – next to some heat - also corresponds with the production of 0,5 m³ of oxygen, this would be an opportunity to strengthen the business case if oxygen could be monetized.

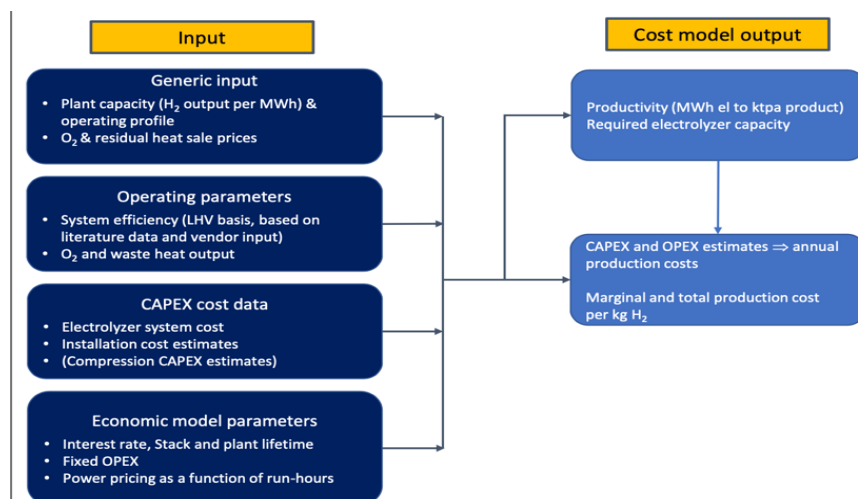
Using proprietary datasets from TNO the capex of the proposed 4,7 MW alkaline electrolyzer has been estimated for an alkaline unit and a – more expensive PEM electrolyzer including installation costs. At this stage the alkaline unit was selected for further evaluation.

An electrolyzer can be operated quite flexibly and may thus make use of favorable electricity prices. The choice of operating hours per annum is therefore an important parameter as it not only impacts the distribution of fixed costs per kg of produced hydrogen (which favors long operating hours), but also the price of electricity as this is not constant over the year (which favors shorter operating hours). As shown in the figure, the lower the hours of operation per annum, the cheaper the price of electricity that could be picked to operate, but at the same time, the higher the fixed costs per hour of production. Picking the right electricity price to operate the unit requires a robust switch-on/switch-off behavior.



For the envisaged an alkaline unit it has been assumed that a minimum operating rate would have to be assumed as the unit is not flexible enough to switch to 0%. Using an actual 2018 electricity pricing profile an average electricity price could be established for the economic evaluation. Electricity costs could be reduced somewhat by playing a role in grid services. This has also been investigated.

Economic evaluation of various options has been carried out by using a model such as pictured below.



By modeling the levelized cost of hydrogen produced, taking into account the potential value of O₂ and heat, at various CAPEX and OPEX pricing a number of Hydrogen cost price-scenarios have been evaluated for the 4.7 MW electrolyzer option.

The base-case has been established for an alkaline unit with 75% utilization per year at 4.7 MWe input, thus yielding a production of 0.59 kta of H₂ (and also 4.73 kta of O₂). The resulting hydrogen price includes CAPEX charges, fixed OPEX charges, variable OPEX charges, benefits from selling heat and O₂ as well as estimated cost of transportation of hydrogen to another location. The latter would assume compressed truck-transport at 350-700 bar and also include compression costs from 30 to 700 bar at AVR. Compression would require a compressor, high pressure storage facilities and truck loading facilities and would hence further increase the cost per t of H₂ somewhat. The overall results show, that even for a relatively small size the variable OPEX cost (mainly electricity) are the largest contributor to the hydrogen costprice albeit that CAPEX contributes also significantly.

At the calculated prices for hydrogen it is not possible at this stage to compete directly with conventional fossil based ("gray" or "blue") hydrogen sources, with costs closer to 1-2 €/kg. The best

hydrogen outlet to be compared with would be the mobility sector although retro-fitting trucks or cars to fuel cell technology, and adjusted pump stations need to be taken into account to allow for hydrogen use. This implies that at current production prices, hydrogen as fuel would still need a significant tax relief or subsidy to compete with conventional fuels.

Due to its higher flexibility, the PEM technology – albeit more expensive - would be able to operate at 0% capacity, which would reduce the average power price per annum somewhat.

2.2 Investigate a 100 MW Electrolyzer to produce merchant hydrogen

The learnings of the more detailed study for the 4.7MWe case have been used to assess the economic impact of scaling up to 100 MWe for use in 2025. Such unit would be able to produce about 12.6 kta of hydrogen and require a plot space of 3000-4000 m². In order to achieve this, some guidelines from suppliers and technology consultants were used by TNO that indicate that CAPEX/MWh would be significantly reduced by 2025 as compared to 2020 by automated production, larger scale and cheaper technology (noble metals).

It is also assumed that engineering scaling rules apply to the price (P) of the electrolyzer equipment (factor f1):

$$P(100MWe) = P(4.7MWe) * \left(\frac{100 MWe}{4.7 MWe}\right)^{f1}$$

and factor f2 for costs of installation (I):

$$I(100MWe) = I(4.7MWe) * \left(\frac{100 MWe}{4.7 MWe}\right)^{f2}$$

The results for a 100 MW facility show that the CAPEX incl installation for a 100 MWe facility – producing 0.59 kta of hydrogen – would indeed be significantly higher than that of a 4,7 MWe facility.

In addition to sheer scale advantages - that reduce the capital cost per ton of H₂ - also developments are expected (see the figure below) between now and 2025 in increasing electrolyzer efficiency for alkaline units and even higher for PEM units. This would further significantly reduce the operational cost per kg of hydrogen. Finally, suppliers expect to maintain electrolyzer efficiency across an ever longer life-span thus reducing CAPEX charges per annum. Both PEM and alkaline units are expected to be able to deliver at higher pressures which will reduce the cost of compressing hydrogen and oxygen prior to further use.

On the basis of above developments and design rules an economic evaluation for a 100 MWe alkaline electrolyzer (producing ~ 2 t/hr of hydrogen or ~15.3 kta based on 85% utilization (which is higher than the 4,7 MWe case) has been carried out. Note that the 100 MWe unit is expected to be more efficient in 2025 and thus yields less waste heat. It should also be noted that – contrary to a small unit - the additional electricity demand would require an extra connection to the grid and possibly major expansion of site-infrastructure (cooling water, pipelines etc) the cost of which have not been taken into account.

As shown by the calculations the compounded effect of scale, production efficiency gains and increased runlength, such unit yields a bare production cost of hydrogen that is much lower per kg than the 5 MWe unit, yet still much higher than the current commercial hydrogen prices. The difference is mainly caused by much lower CAPEX charges (with the said caveat that major adjustments of site infrastructure at AVR have not been captured) as electricity costs per kg of H₂ will be similar as, despite somewhat better efficiency, the average MWe price per kg of H₂ will be higher

due to the longer run-length per annum. In this case only part of the associated oxygen has been assumed to be sold to Tronox who have a need for less.

Note that in case only pure green hydrogen would be targeted, the electricity supply would have to follow the availability profile of wind-electricity, which is typically around 4800 hrs per annum. Such operating hours would give a more interesting electricity price but much higher CAPEX charges.

2.3 Investigate chemical routes to monetize AVR H₂ and Tronox' CO-rich streams

Next to AVR selling merchant hydrogen for conventional chemical processes such as hydrotreating or as fuel, it could also be envisaged that Tronox' proximity plays a further role than the evaluated uptake of oxygen as extra the valorization of hydrogen.

Two alternative routes have been investigated that make use of Tronox and AVR assets:

Route 1

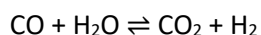
Producing additional hydrogen from available process-CO at Tronox. Additional hydrogen could be generated at Tronox by removing CO₂ from a CO-rich gas-stream at Tronox using an amine unit to remove CO₂ and shift the remaining CO with water to produce hydrogen and additional CO₂. The proprietary TNO SEWGS© technology would enhance this route by removing CO₂ during the process.

Route 2

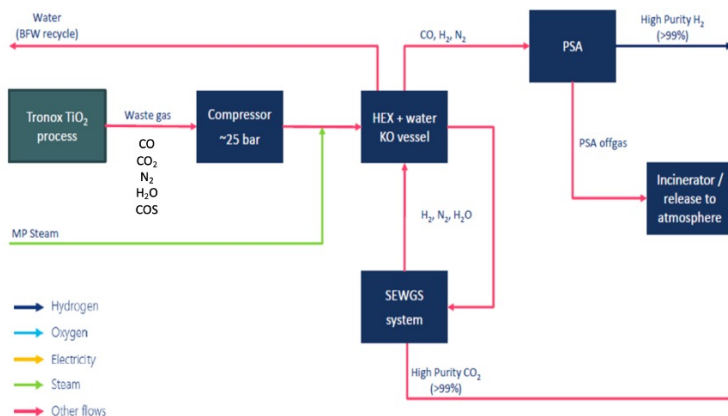
Using CO from Tronox to produce methanol with AVR's hydrogen. To this end hydrogen is added with Tronox' CO/CO₂ gas to produce syngas (a mixture of CO/H₂), which is a feedstock for the production of methanol.

2.3.1 Converting CO to produce additional hydrogen and capture the CO₂

TNO's SEWGS© (sorption enhanced water-gas shift) process is an integrated water-gas shift and CO₂ capture process. Roughly 95% of the CO₂ already present in the waste gas stream, and the additional CO₂ that is produced, is captured in a CO₂ stream with a CO₂ purity of >95% (dry basis). The SEWGS© route to produce hydrogen from CO removes CO₂ that is produced during the reaction (at ~400 °C) via absorption and hence shifts the equilibrium to maximise hydrogen production.



The CO₂ is removed from the reaction mixture via a CO₂-selective sorbent using a pressure-swing system: CO₂ is selectively absorbed from a gas-mixture at high pressure and - once saturated - desorbed at a lower pressure. After absorption of CO₂, the remaining CO reacts with added steam to yield hydrogen and new CO₂ – which is again absorbed. The residual mixture of hydrogen (and unfortunately in the case of Tronox also quite some nitrogen) is separated downstream in a conventional Pressure Swing Absorber downstream of the SEWGS© unit. Downside is that the gas-stream needs to be compressed to about 23-25 bar to allow the physical separation of CO₂ to take place.



In order to economically quantify the above process, it was assumed that Tronox off-gas is currently routed to an incinerator with additional natural gas to produce modest amounts of steam and a diluted CO₂ stream. Not all CO present would be converted to H₂ due to some downstream PSA losses.

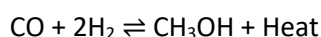
Since the production of hydrogen is only modest, similar order of magnitude as the 5MW electrolyzer, and the key product would be concentrated CO₂, it makes sense to evaluate this route as a CO₂ capture route with (blue) hydrogen as a valuable by-product. The alternative route to remove the harmful CO and currently applied at Tronox is incineration with additional natural gas and air to produce a mixture of approximately equal amounts of CO₂ and nitrogen that is currently vented. Post-combustion CO₂ capture technology could be applied to reduce CO₂ emissions from the stack of the incinerator, but this option was not in the scope of the current study.

The associated economic evaluation looked at CAPEX, fixed OPEX, variable OPEX and hydrogen benefits. It showed that for Tronox scale this would be an interesting decarbonization route when compared to the alternatives such as amine treating.

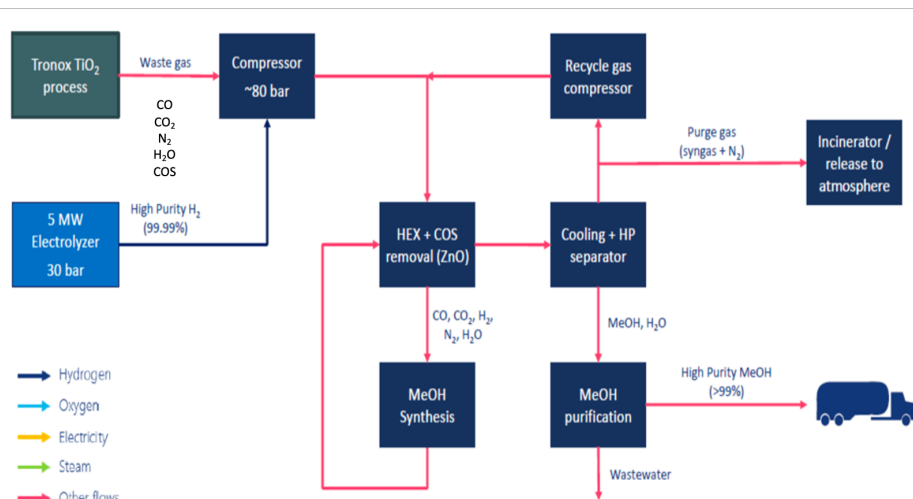
2.3.2 Converting CO from Tronox to methanol, using H₂ produced at AVR

This final case is linked to the existence of a 100 MW electrolyzer at AVR, which would make ~15 kta of hydrogen available to convert most CO and some CO₂ from the Tronox gas into methanol.

The selected process, based on Tronox' full residual gas flow, has been pictured below. The process uses CO from Tronox and converts this to syngas with AVR hydrogen. This subsequently produces >99% pure methanol at about 80 bar and 250 °C in the presence of a Cu/Zn/Al₂O₃ catalyst according to the following reactions (after removal of COS using ZnO):



Due to the equilibria and low conversion, the reaction requires a very significant recycle of non-reacted CO/H₂ which also implies a significant purge to avoid build-up of inert materials (for example Nitrogen present in the Tronox gas). The formed methanol is removed via cooling and led into a distillation section. The gases are recycled.



For the economic evaluation the CAPEX included the MeOH synthesis reactor, sulfur removal unit and compressors. Furthermore the Hydrogen-price would be derived from the 100MW case for delivery at higher pressure and the purge rate would be estimated.

The economic evaluation (see figure below) yielded the following results:

- (i) Methanol produced at this scale and in this way would cost significantly more than the typical market value, based on natural gas reforming or coal gasification, which would fluctuate between 150-400 €/t.
- (ii) By far the most expensive part would be the cost of hydrogen and even at current hydrogen prices (1.5 €/kg for “blue” hydrogen) this scale would prohibit economic feasibility.
- (iii) Process economics would be improved by reducing the concentration of N_2 and/or by increasing the pressure of the off-gas from Tronox.

3 Potential CO₂ reductions

The e-Thor study has evaluated four concepts, with different impact in terms of CO₂ mitigation. Hereunder some high-level estimations of the CO₂ impact have been discussed. It is, however, recommended to carry out an LCA to properly evaluate the impact for the selected case.

The 5 MW demo for H₂ production via electrolysis would produce around 0.59 kta of hydrogen using electricity. The average power generation footprint in the Netherlands could be used as a first estimate. This is currently 0.475 t CO₂ /MWh (<https://www.co2emissiefactoren.nl/lijst-emissiefactoren/>). Using AVR's electricity for hydrogen production today (52.3 kWh per kg H₂ required) would actually increase the overall CO₂ emissions. In case the power balance would be restored elsewhere via green electricity or in case AVR would use excess power the picture would be different.

If AVR hydrogen would be used for mobility (cars, trucks, small vessels) every kg of H₂ would displace roughly 5 l of diesel, equivalent to ~ 13 kg CO₂ emissions. The annual production of 0.59 ktpa H₂ could therefore save up to 7.7 kt CO₂/a in road transport related emissions.

Increasing the scale to 100 MW full-scale H₂ production (about 15 kta) would change the picture, as it is to be expected that the alternative use of power by AVR would impact the supply-demand balance. Only in case the CO₂ footprint of the grid would be significantly reduced – or when bringing extra dedicated green electricity to replace AVR's share - such case could yield an overall CO₂ reduction. At this scale a logical replacement would be displacing Steam Methane Reformed (SMR) H₂ in the refining sector, where for every ton of H₂ currently about 8.5-9 ton CO₂ is emitted. Using AVR's hydrogen would therefore potentially avoid a maximum of ~135 kta of CO₂ emissions – provided AVR's void would be filled with green electricity.

The case of conversion of CO byproduct from Tronox to hydrogen via the SEWGS® technology and yielding 100% pure CO₂ which can be directly compressed and sent to a CO₂ trunk line for storage rather than incineration waste gas is indeed a clear-cut CCS case. It would lead to a reduction of ~82 ktpa CO₂ emissions from the Tronox site. If the (blue) H₂ produced displaces SMR hydrogen, an additional indirect reduction in the order of 6.5 ktpa CO₂ can be achieved.

The final case, methanol production from Tronox waste gas, would convert more than half of the CO₂ emissions (nearly 50 ktpa) from waste gas incineration at Tronox into methanol. If the methanol is used as a fuel, the CO₂ will be emitted but emissions from conventional methanol production will still be offset. Using the methanol produced in this case as a chemical building block will increase the impact in terms of (short-term) emissions reduction.