METROLOGY for HYDROGEN VEHICLES

HYDRAITE

Impurity risk assessment model

Jari Ihonen (VTT)

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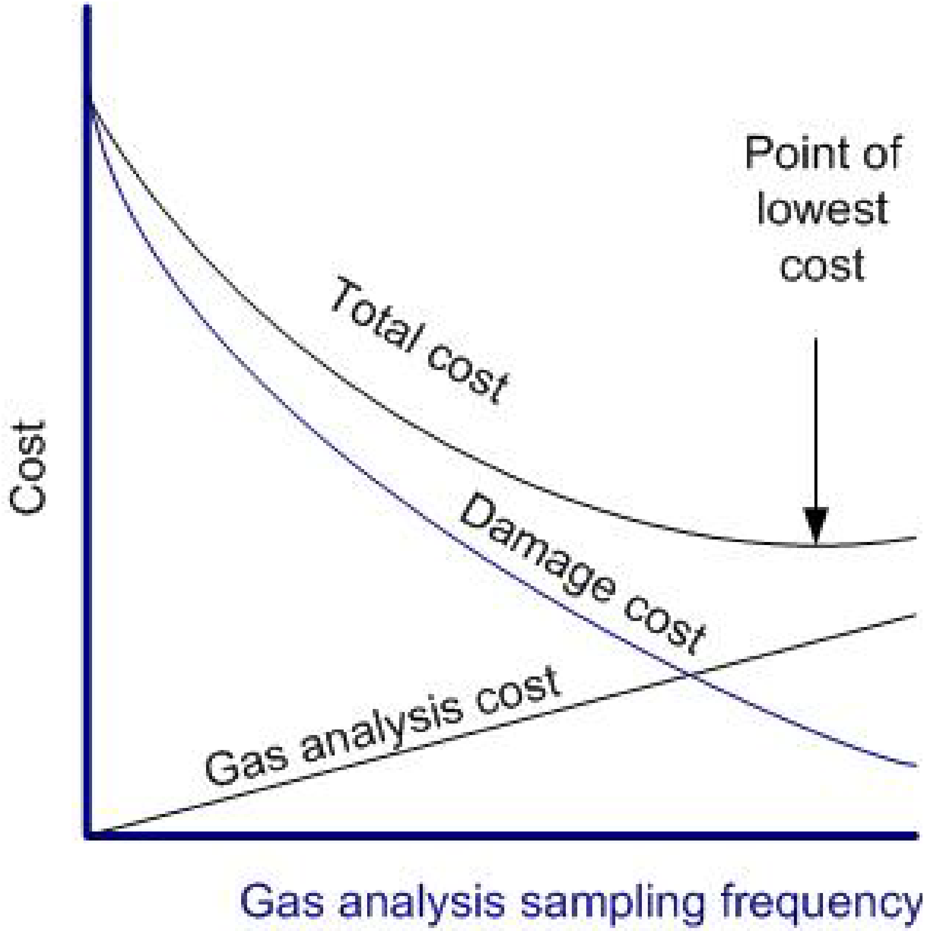
EMPIR EURAMET FCH

Overview

- The challenge
- Introduction to the risk assessment model developed in HyCoRA project
- Development of the risk assessment model in HYDRAITE project
- Result example from HyCoRA project

Modelling challenge - the cost of automotive grade hydrogen is too high

- For large scale commercialisation of FC vehicles (inc. trains, ships) hydrogen delivered to retail station should be under 5 € / kg in the long term
- In most of the current HRS, expensive hydrogen is delivered from sources with very low risk in order to fulfil requirements of ISO standard
- In the commercialisation phase of FCEV low cost hydrogen sources should be utilised.
- A cost optimisation model is needed



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Introduction

HYDRAITE/HyCoRA strategy – quantitative risk model

- The HyCoRA quantitative risk model is based on analytic approach of probabilistic risk. The model defines the probabilistic coupling between the harmful effects on PEMFCs and FCEVs that impurities in hydrogen fuel introduced at refuelling may induce.

- Risk assessment provides information for the required frequency and accuracy for the gas analysis at the nozzle and/or in production

- Risk assessment gives **the right focus** for development of the **new analytical methodology for the gas analysis**

Risk assessment requires information from:

a) the real susceptibility for various poisonous species specifically for automotive applications – automotive type FC system data needed

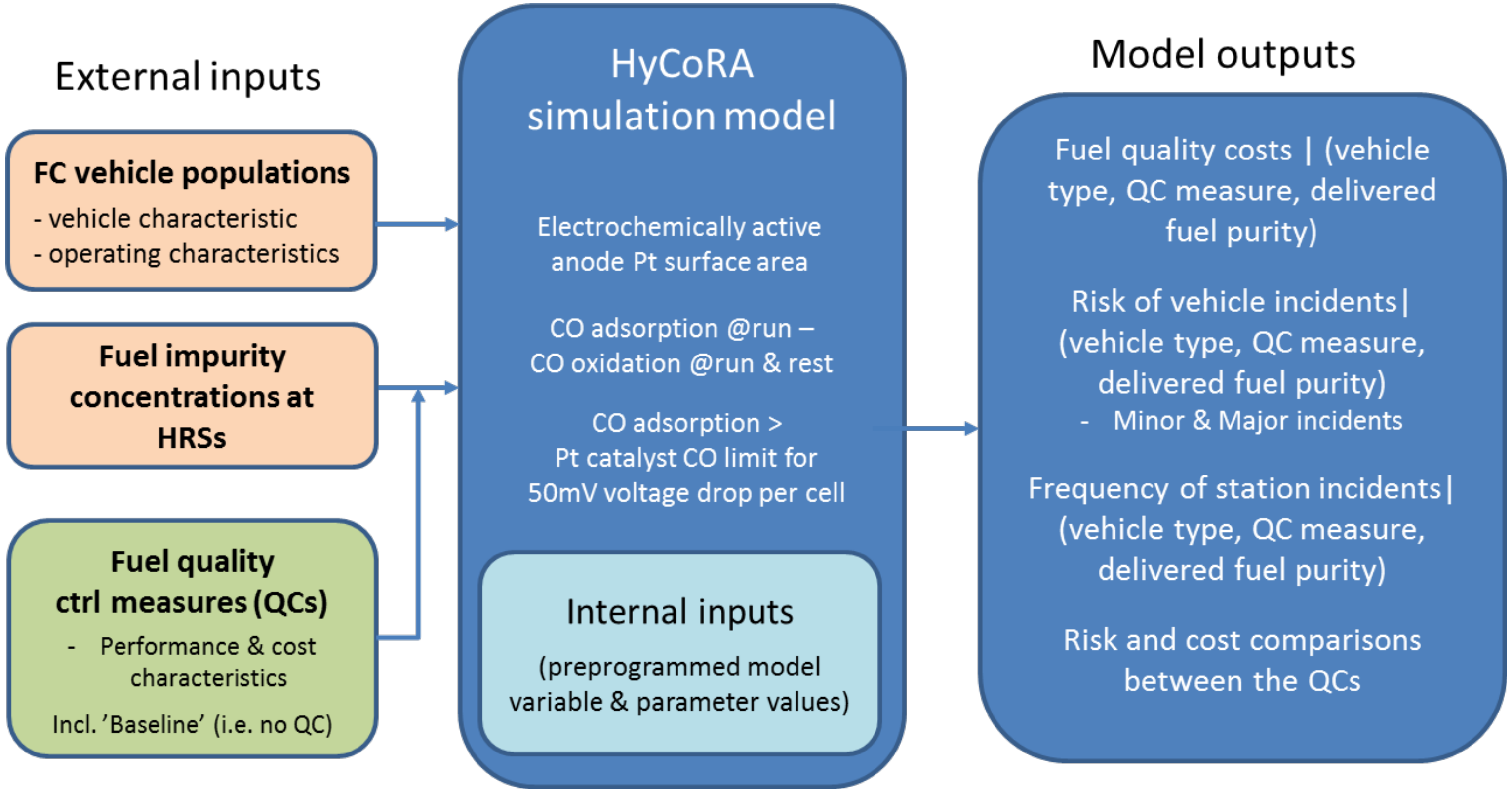
b) probabilities for quality assurance QA failure in hydrogen production site and/or at HRS – data for gas analysis methods needed

c) probabilities for introducing contaminant during delivery and dispensing of hydrogen at HRS

d) concentration correlations between contaminant species in fuel - impurity concentrations at production sites and HRS nozzle needed

Model and assumptions

HYDRAITE/HyCoRA concept for fuel quality risk & cost simulation – CO adsorption is the key parameter



- Monte Carlo simulation applied to deal with and process the various sources of uncertainty involved
- Population of HRSs used by a population of FCEVs
- ***Every FCEV refilling poses a risk situation (i.e. possibility for contamination by fuel impurities)***

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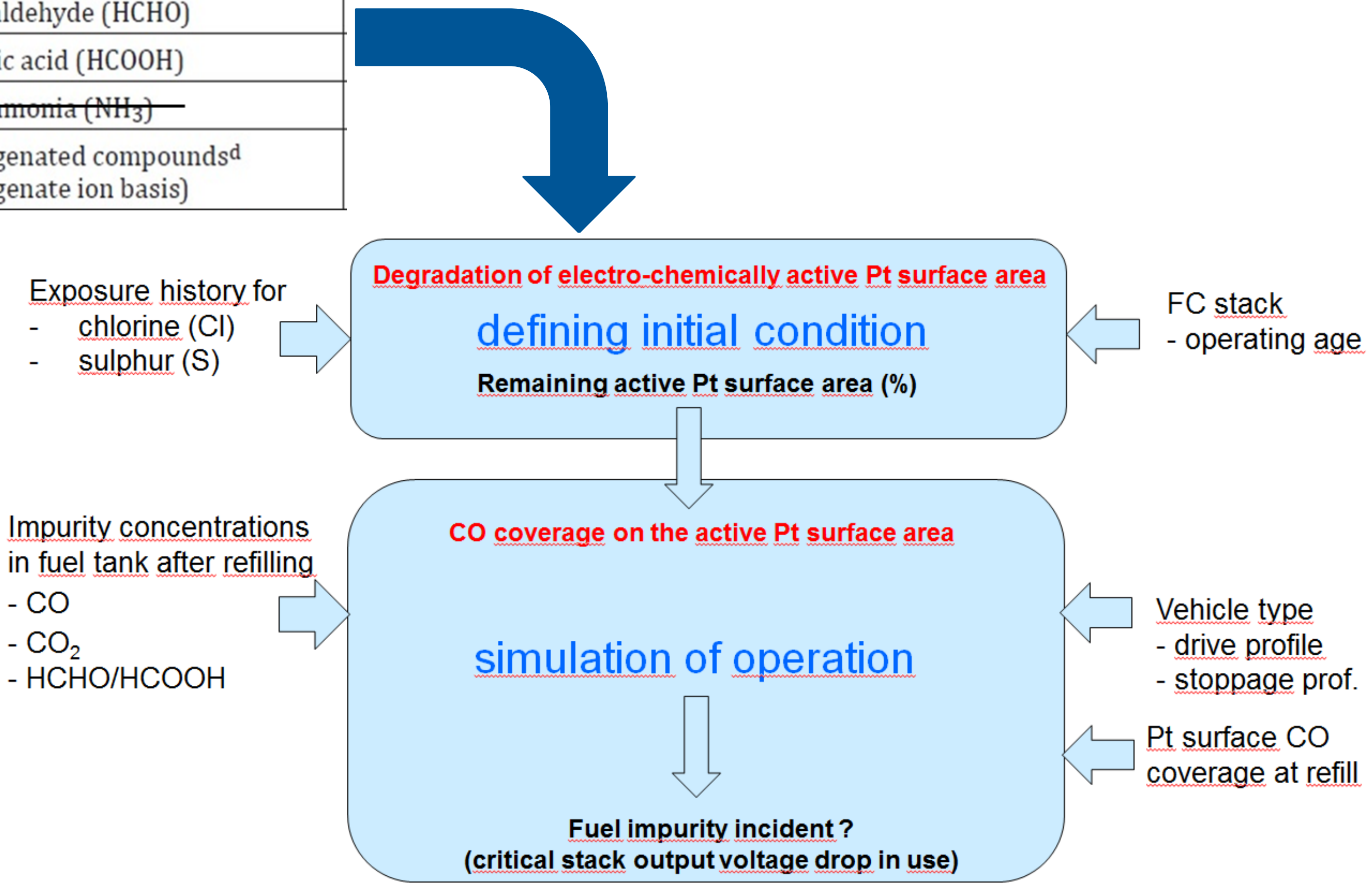
Relevant fuel impurities and the impact mechanisms

- The formation of CO on the surface
- The formation of CO on the surface
- The loss of available area due to almost irreversible adsorption of S
- The formation of CO on the surface*
- The formation of CO on the surface*
- No effect on the anode, but on the cathode (Hashimasa 2011)
- Accelerates the particle growth and Pt area loss – how much on the anode?

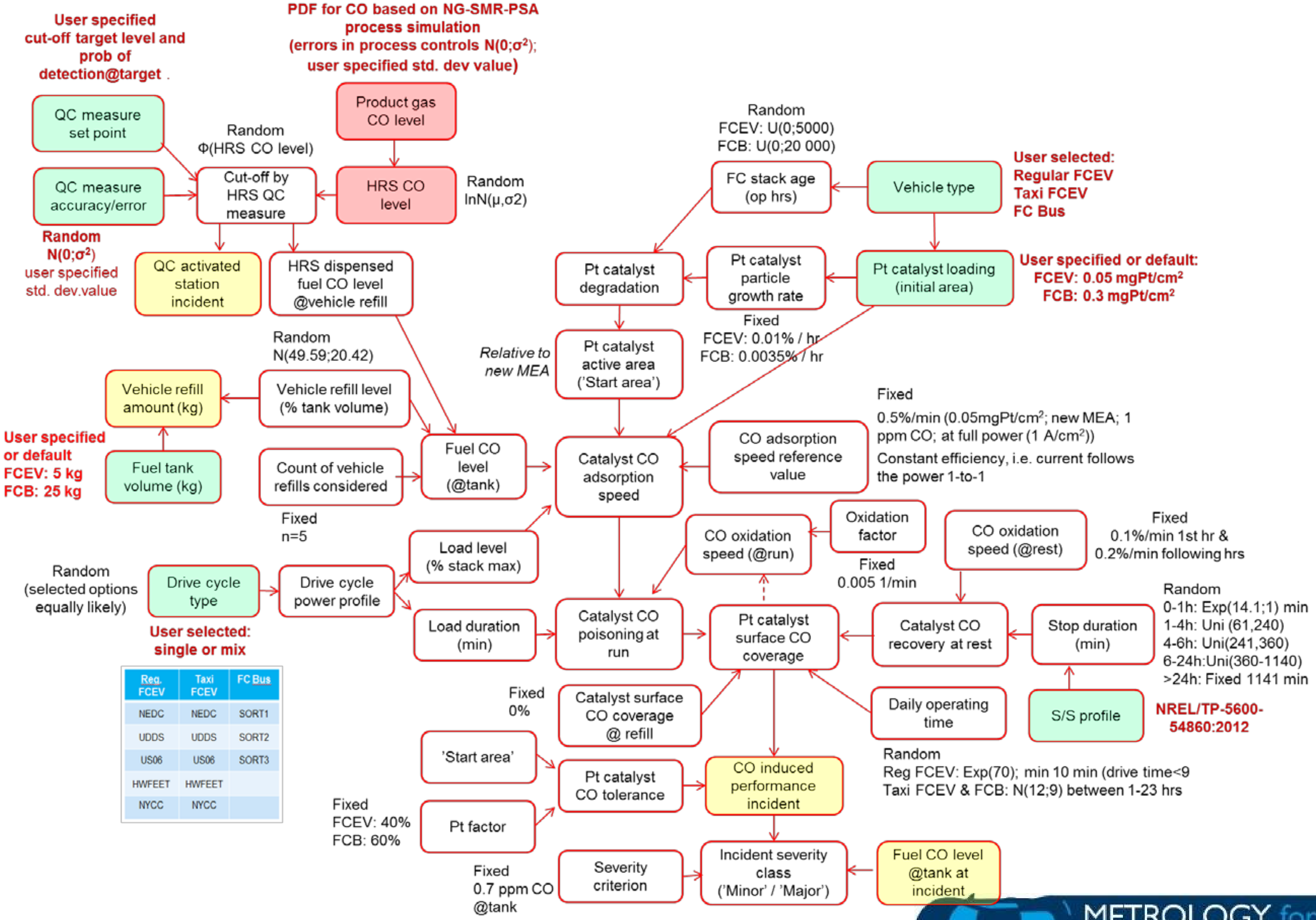
Carbon dioxide (CO_2)
Carbon monoxide (CO)
Total sulfur compounds[c] (H_2S basis)
Formaldehyde (HCHO)
Formic acid (HCOOH)
~~Ammonia (NH_3)~~
Total halogenated compounds[d] (Halogenate ion basis)

Two impurity impact mechanisms of **different time scales** separated:

1. degradation of electrochemically active anode Pt surface area (**FC age**; S and Cl- species). Time scale years.
2. active Pt surface area **contamination by CO** in vehicle use (fully recoverable). Time scale hours (HyCoRA) or days (HYDRAITE)



Model variables and currently applied values: ’CO only’ v1.0



Reg. FCEV	Taxi FCEV	FC Bus
NEDC	NEDC	SORT1
UDDS	UDDS	SORT2
US06	US06	SORT3
HWFEET	HWFEET	
NYCC	NYCC	

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HYDRAITE / HyCoRA fuel quality risk & cost simulation model

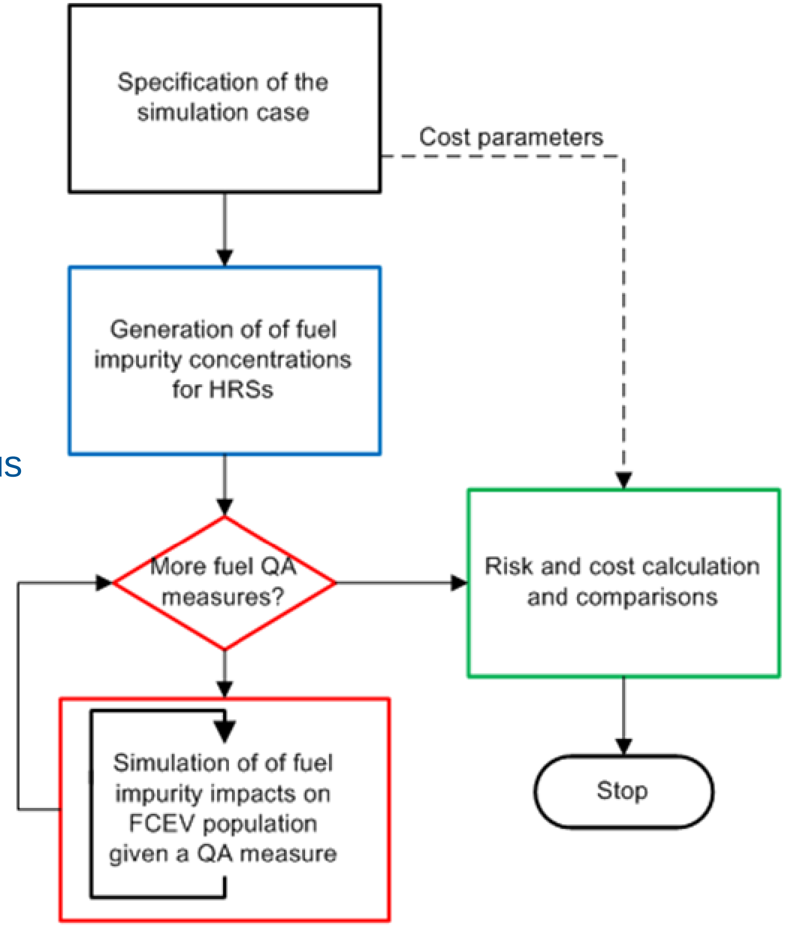
- Select vehicle type & use
- Specify initial Pt loading
- Select fuel source
- Specify QC measure(s)
- Define calc. parameter values

Generate probability distributions for impurity concentrations in fuel delivered to HRSs

Identify QC measures for continuous online monitoring of fuel impurities

Expose population of vehicles to driving with fuel conditioned by specific QC measure

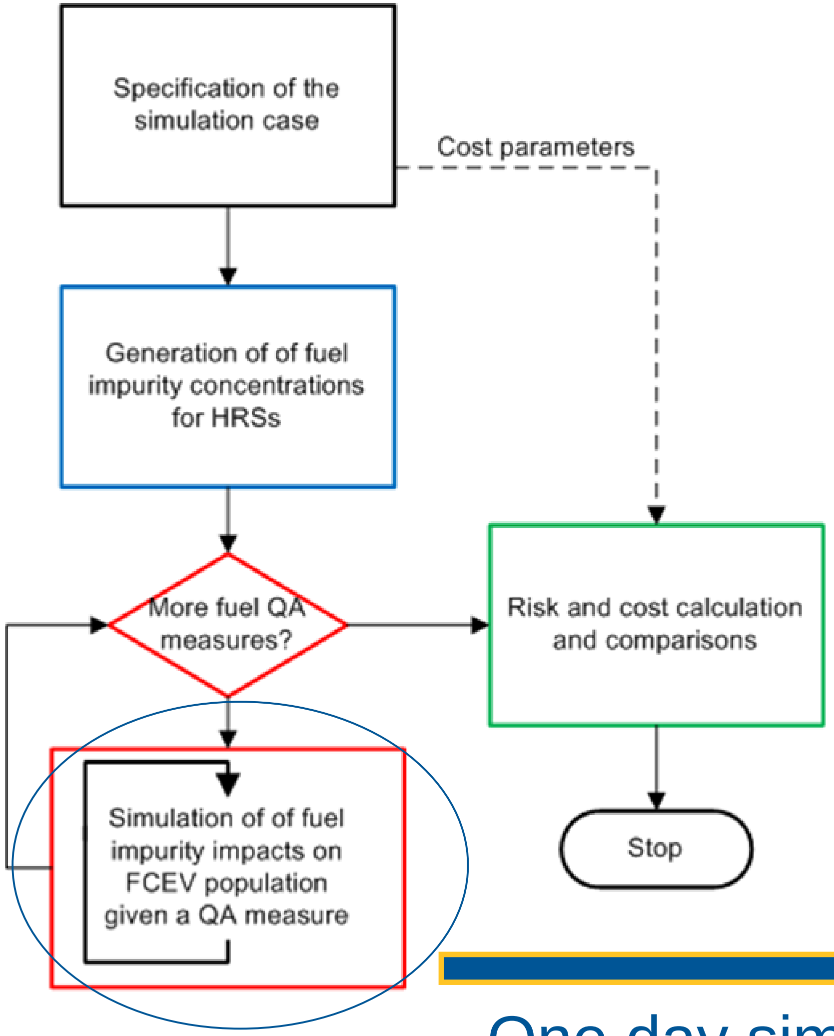
- random vehicle
- refill at random HRS
- daily operation according to selected drive cycle type (single or mix), random stoppage times and random daily operating time

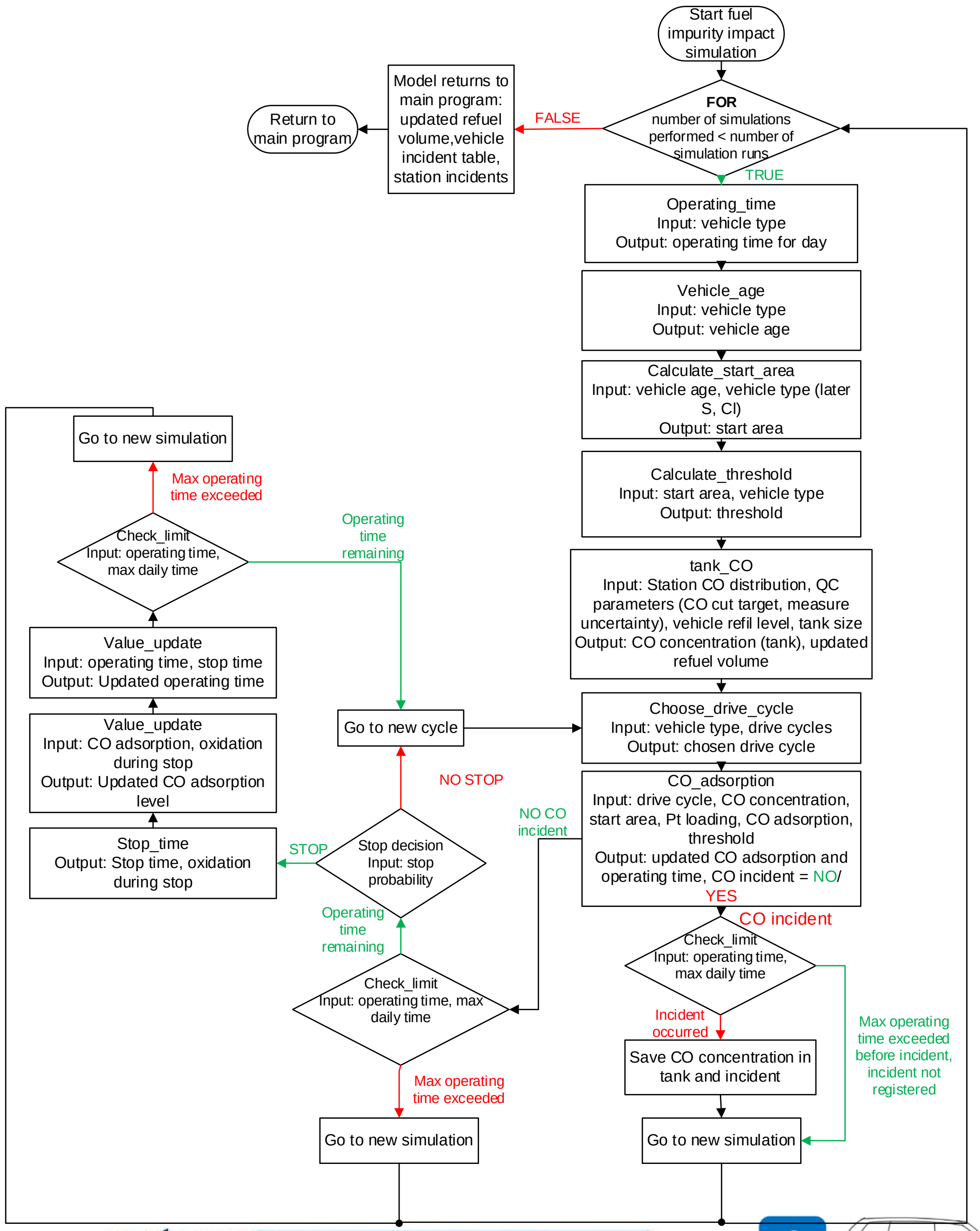


- Likelihood of vehicle incidents given the QC measure
- Cost impact of QC measure
- QC measure minimizing the fuel quality cost

Total cost (€/kg) | QC_i =
capital & operating costs of QC_i
+ cost of vehicle incidents|QC_i
+ costs of HRS incidents|QC_i

HYDRAITE/HyCoRA Matlab model, - flowchart





One day simulations now

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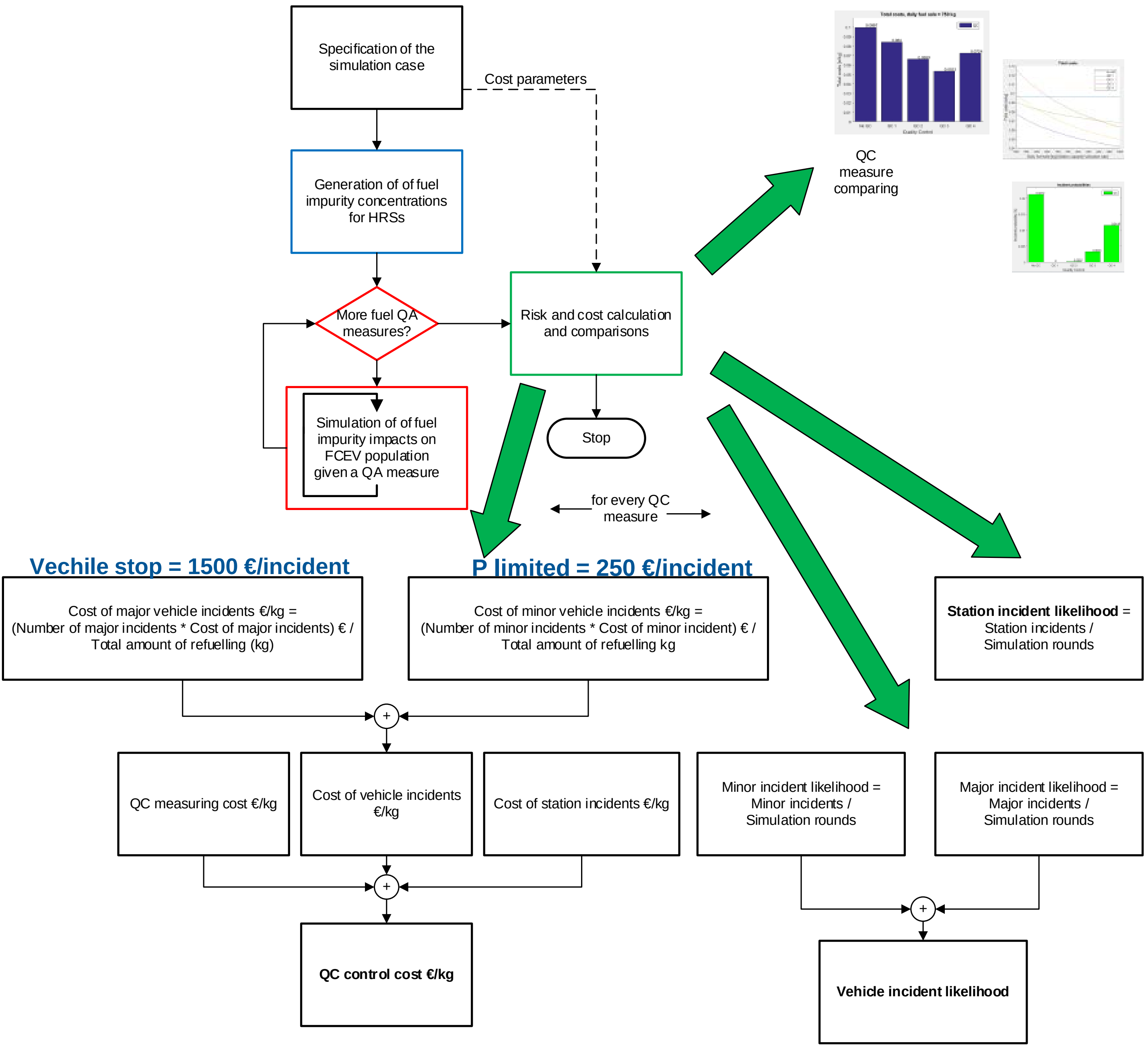
Risk and cost calculations

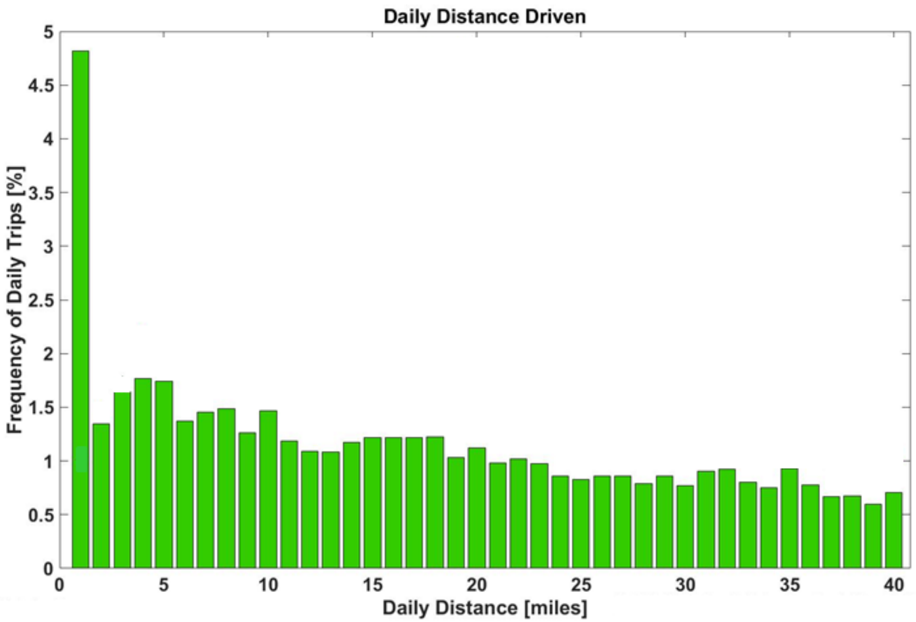


Limitations & uncertainties in versions 1.0
- > and improvements for model 2.0

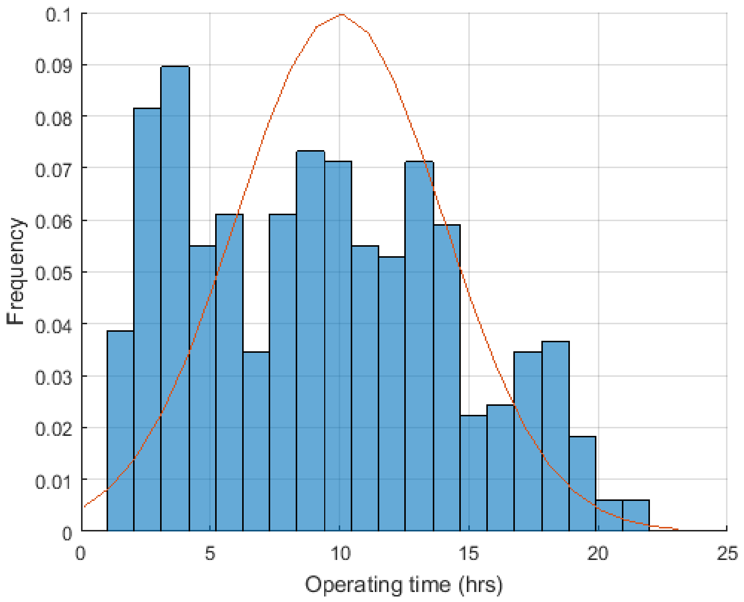
- Only **age related degradation** of the active Pt surface area accounted; - > S will be included, maybe Cl-
- CO only reversible fuel impurity considered - > CO_2 will be included
- SMR-PSA only hydrogen production method considered (data simulated) -> real SMR-PSA data and other production methods
- Vehicle operating profiles based on NREL data – relevance to real operation? -> improved NREL data, data from EU demos (ZSW)
  - model outputs sensitive for changes in drive cycles, stoppage time distribution, operating time distribution
- CO adsorption reference value based on 0.05 mgPtcm-2 Pt loading and maximum current density 1 Acm-2 -> more choices will be added
- System efficiency assumed to be constant, i.e. current follows the power 1-to-1 –> will remain until reliable data available
- 50 mV voltage drop per cell applied as the limit for failure –> will remain, if not new input from OEM
- CO oxidation rates at stop based on semi-open cathode –> more data about H_2 soak stop, **from one day to much longer** simulation time
- CO oxidation rates at run and at stop assumed to remain constant over system life –> more data from FC measurements
- Lack of accurate cost data –> better estimates for all cost and damage values

Results from model 1.0 simulations

Estimated vehicle user profiles for regular FCEVs and taxis



Daily drive distance distribution for regular FCEVs



Daily operating time distribution for FC Buses and taxis

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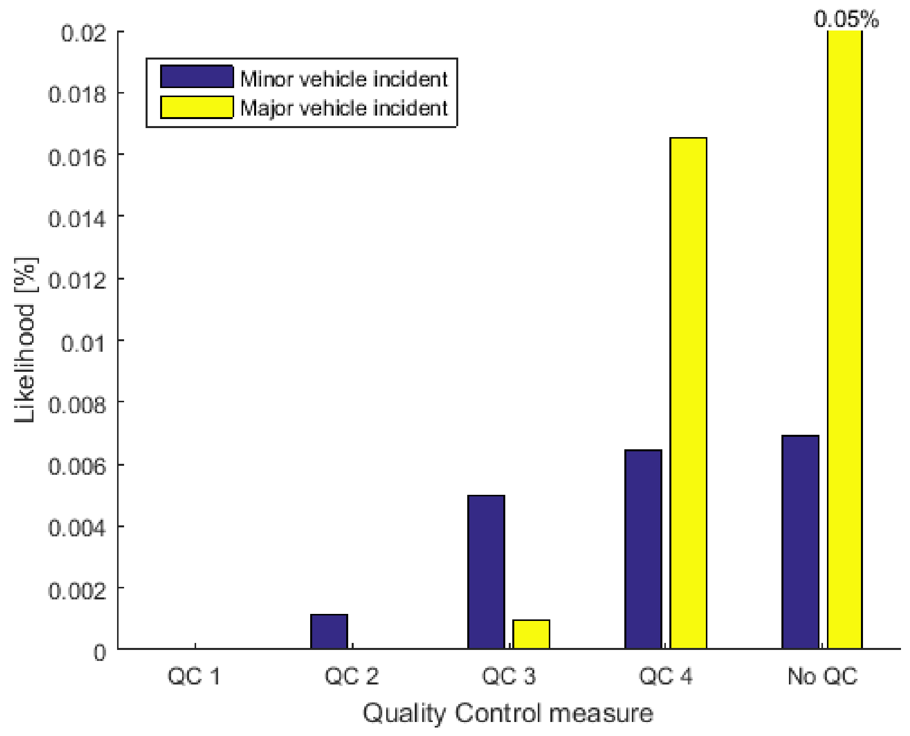
Assumptions about instrument costs

1: Papadias et al, Int J Hydrogen Energy 2009;34:6021–35
2: Best estimates for instruments in 2017

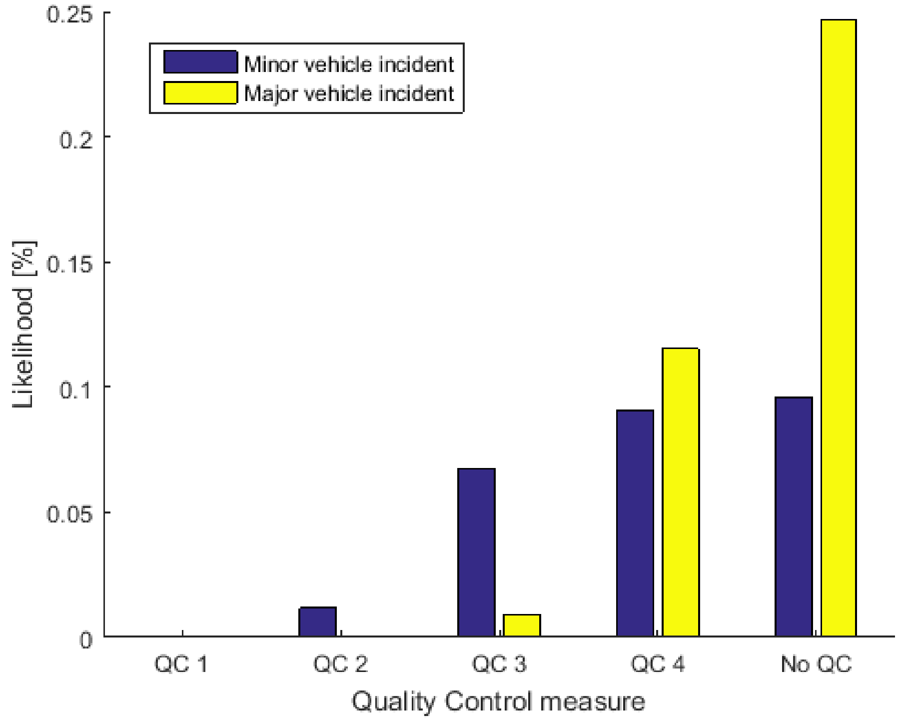
QC name	QC 1	QC 2	QC 3	QC 4	No QC
CO cutoff target (ppm)	0.2	0.5	1.0	2.0	n/a
Measurement error (ppm)	0	0	0	0	n/a
Probability of detection at target	1	1	1	1	n/a
Instrument cost 1 (€)	100 000	75 000	50000	25000	0
Instrument cost 2 (€)	50 000	25 000	15 000	5000	0
Instrument life (years)	5	5	5	5	n/a
Maintenance (€/year)	3000	3000	3000	3000	0

Note: 50 k€ instrument with LoD 30 ppb or even much lower could be possible in 2017

Likelihoods of experiencing minor or major incidents in Regular FCEVs and Taxi FCEVs - for taxis much more incidents



Regular FCEV



Taxi FCEV

(notice different scale)

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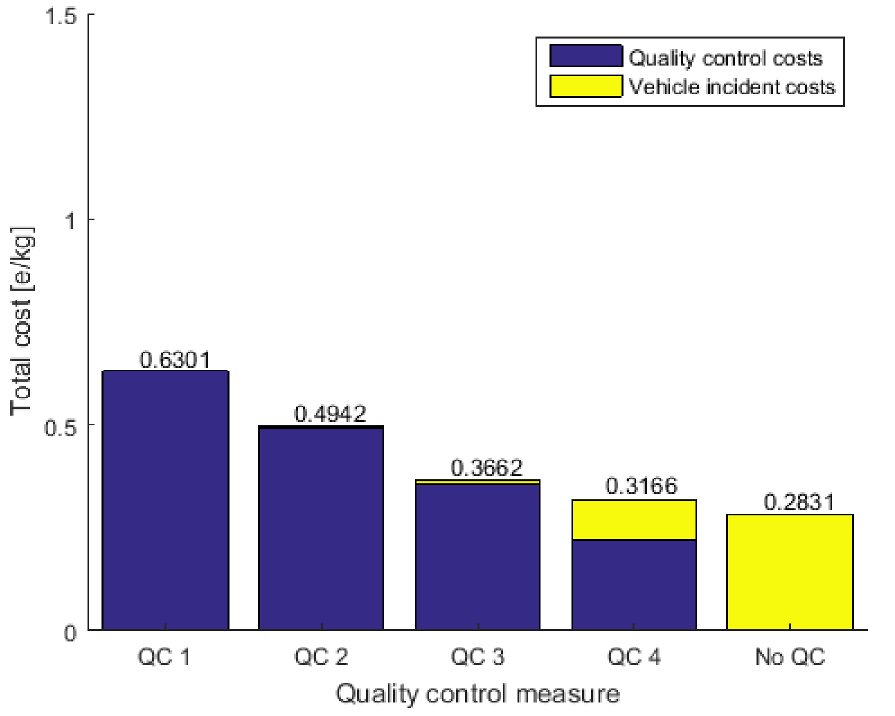
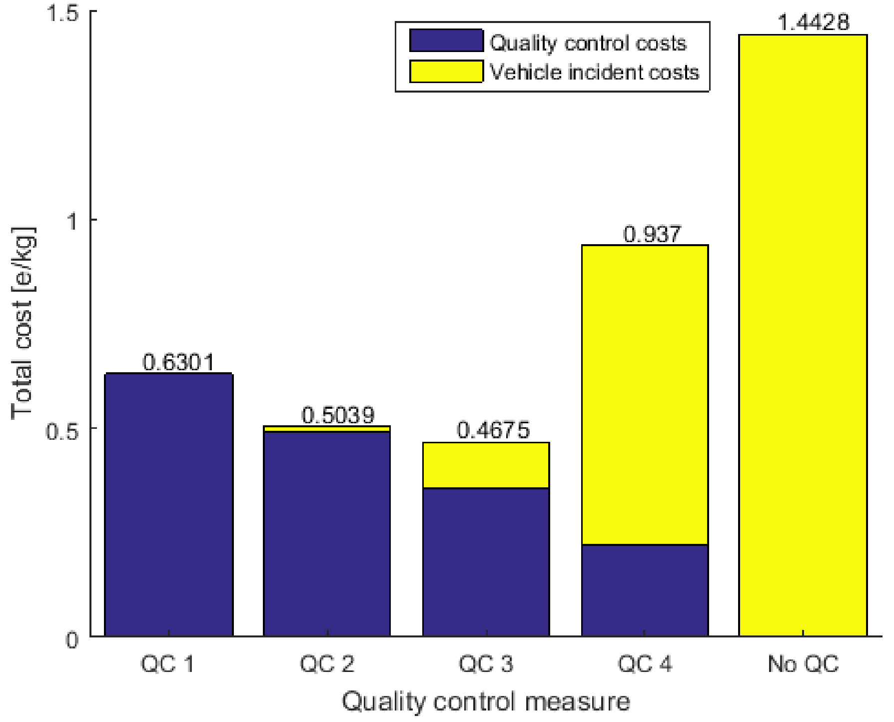
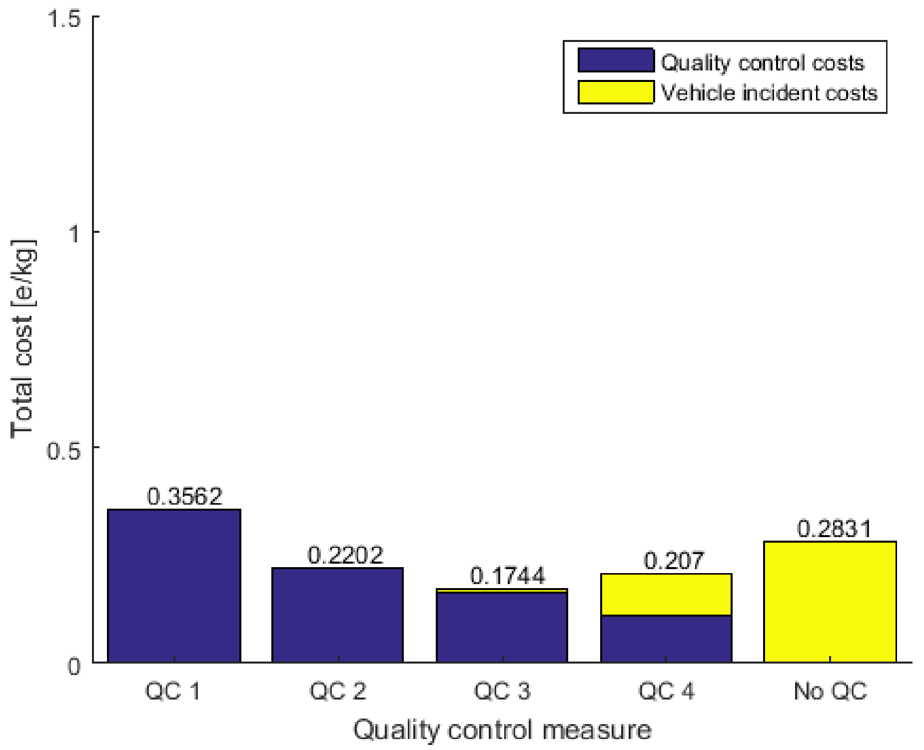
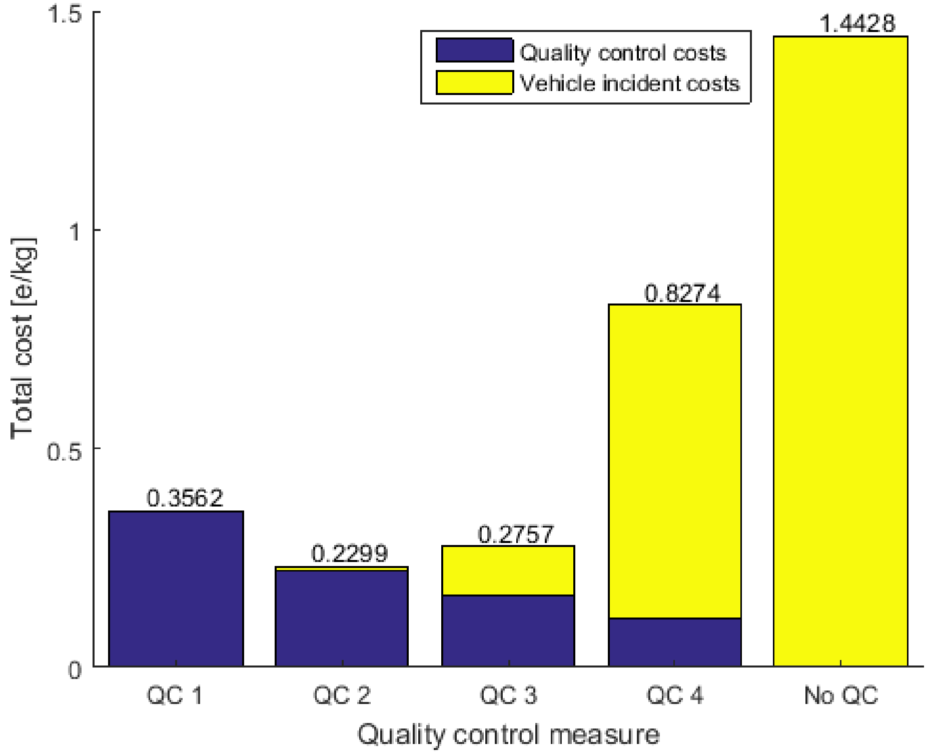
Total cost of the different QC options, instrument cost 1 (higher), HRS daily sales volume 100kg – for taxis better control needed

	
Regular FCEV	Taxi FCEV

Total cost of the different QC options, instrument cost 2 (lower), HRS daily sales volume 100kg – some control always good idea

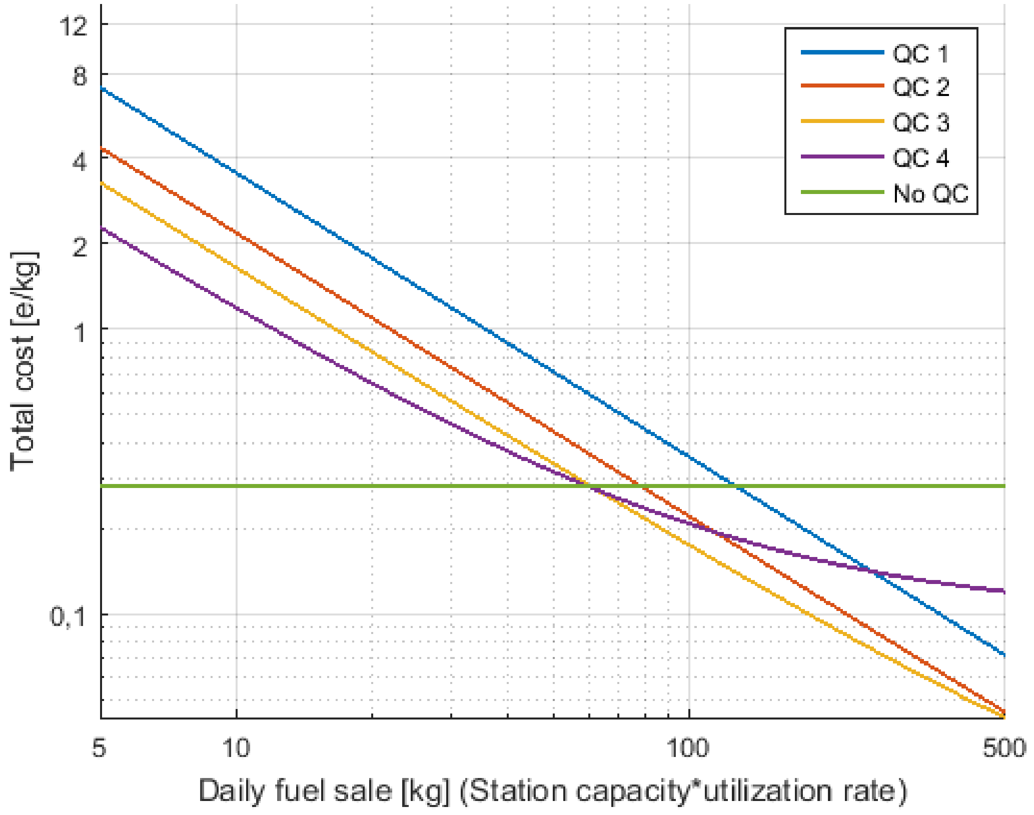


Regular FCEV

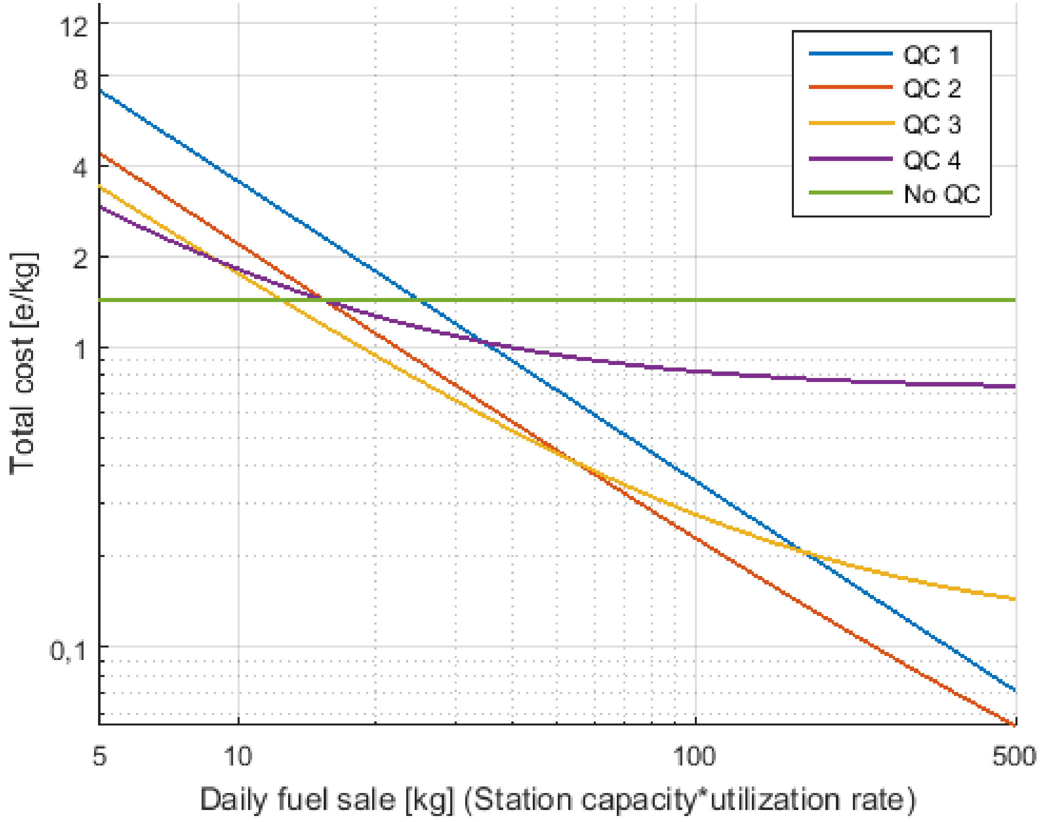


Taxi FCEV

Total cost of the different QC options, instrument cost estimates 2 – more H2 dispensed, better control needed



Regular FCEV



Taxi FCEV

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Discussion and conclusions

- The risk model developed in HyCoRA project can be used to estimate the most cost efficient QA measures
- QA measures needed are dependent on the expected quality of fuel as well as daily delivery of fuel
- On-line monitoring of CO at HRS will become the most cost efficient solution if instrument costs can be reduced
- Preliminary result shows that with LoD 0.2 ppm **all** CO based vehicle incidents can be eliminated.

Available resources

- HyCoRA reports, : http://hycora.eu/deliverables.htm
  - D4.3 Final risk assessment of hydrogen fuel quality assurance methods

- Article:
- Tuominen, R., et al (2018) International Journal of Hydrogen Energy, 43 (9), pp. 4143-4159.

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THANK YOU

Jari Ihonen

jari.Ihonen@vtt.fi

+358503460970

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