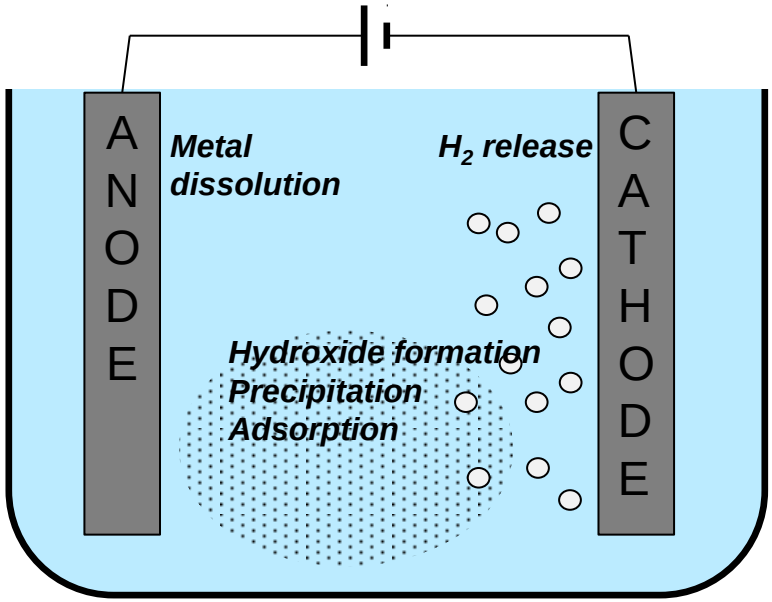
Virtual Upscaling
EWT process modeling

Mikko Manninen, Ulla Ojaniemi
VTT CFD Modelling

EWT-process



- Anode
  - Dissolution of metal ions by oxidation
- Cathode
  - Reduction of water into hydrogen (gas)
- Bulk
  - Hydroxide formation
  - Reactions with pollutants
  - Precipitation
  - Settling (or flotation) of particles

EWT process modeling (1)

- Anode
  - Rate of metal dissolution Faraday's law

    $$\dot{m} = \frac{\phi I M}{Z F}$$

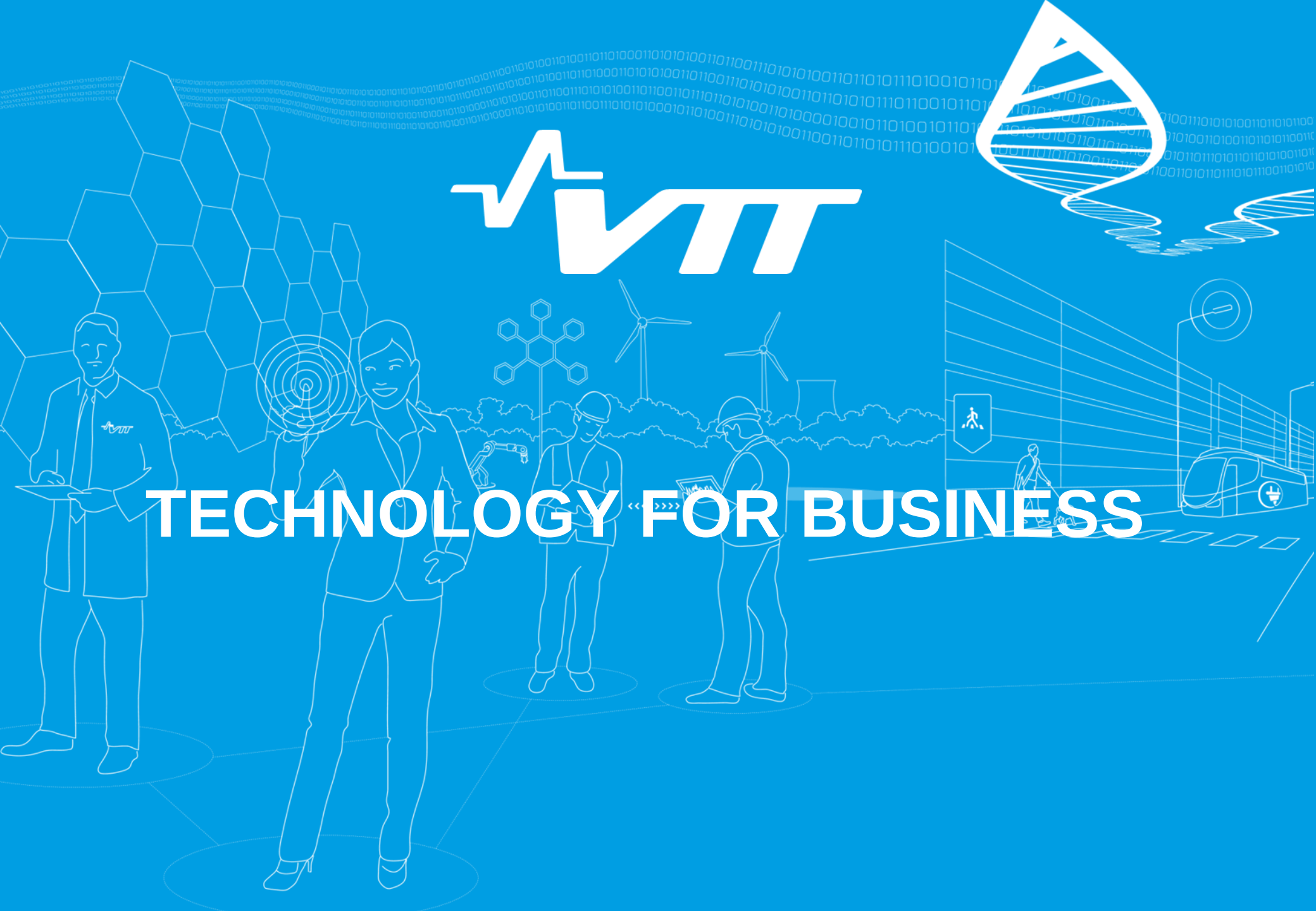
  - Diffusion-convection of ions from metal surface to bulk liquid
  - Thickness reduced – effects on flow etc.
- Cathode
  - Rate of hydrogen gas release determined by the (local) electric current
  - Hydrogen bubble formation – transport by diffusion, convection and buoyancy

EWT process modeling (2)

- Bulk liquid
  - Flow and turbulence
  - Ion species transport (convection, diffusion, electric forces)
  - Liquid phase reactions, fast equilibrium, pH of solution
  - Precipitation of poor solubility metal hydroxides and more complex compounds
  - Solid particle and gas bubble transport (multiphase CFD)
- Constant electric field assumed as a first approximation
  - But current is a local quantity due to spatial variation of conductivity

EWT modeling, CFD-HSC coupling

- Transport of ionic species (liquid phase), particles and gas bubbles is calculated in CFD (Ansys Fluent)
- Thermodynamic equilibrium of ion speciation is solved in HSC locally in every computational cell
  - Interface between Fluent and HSC will be created
- Precipitation is calculated in CFD using nucleation/growth kinetics
- CFD model results are used in improving the accuracy of the system level HSC model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