



Chair of Process Technology and Industrial Environmental Protection

Master's Thesis

Modeling and simulation of the copper
recycling from wastewater in AT&S

Sarah Julia Notter, BSc

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„Man muss die Dinge so einfach wie möglich machen. Aber nicht einfacher.“

- Albert Einstein

Kurzfassung

Modellierung und Simulation des Kupferrecyclings aus Abwässern in AT&S

Die Ziele dieser Masterarbeit sind die Einführung einer Simulationssoftware, die anschließende Entwicklung eines Prozessmodells und eines Simulationsrahmens. Dadurch soll die Einführung und Implementierung der hauseigenen Recyclinganlage von Kupfer und Salzsäure in anderen AT&S Werken vereinfacht werden.

Eine ausführliche Literaturrecherche führt in die Themen Kupfer als Rohstoff, industrielles Abwasser und Abwasserbehandlung ein. Dabei wird auch die AT&S eigene Recyclinganlage detailliert erläutert, die anschließend modelliert wird. Außerdem wird kurz auf die Theorie von Prozessmodellierung und Simulation eingegangen.

Der praktische Teil der Arbeit beginnt mit der Definition der Anforderungen, der Auswahl einer Software und der anschließenden Implementierung von ITHACA. Durch die Sammlung von Prozessdaten der bereits bestehenden Recyclinganlage in AT&S Hinterberg (Österreich) kann ein Modell und ein Simulationsrahmen erstellt werden, um zukünftige Prüfungen der Anwendbarkeit des Recyclingkonzepts zu ergänzen. Die Modellentwicklung, Validierung, Verifizierung und Schaffung eines Simulationsrahmens werden dabei dokumentiert.

Abstract

Modeling and simulation of the copper recycling from wastewater in AT&S

The objectives of this master's thesis are the implementation of a simulation software, the subsequent development of a process model and a simulation framework. This should simplify the roll-out and implementation of the in-house recycling plant for copper and hydrochloric acid in other AT&S plants.

Extensive literature research introduces the topics of copper as a raw material, industrial wastewater and wastewater treatment. Moreover, the AT&S in-house recycling plant is also explained in detail, which is then modeled. The theory of process modeling and simulation is also briefly discussed.

The practical part starts with the definition of requirements, the selection of the software and following implementation of ITHACA. By collecting process data from the existing recycling plant in AT&S Hinterberg (Austria), a model and a simulation framework can be created to complement future tests of the applicability of the recycling concept. The model development, validation, verification and creation of a simulation framework are also documented.

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1 Introduction

1.1 About AT&S

The *Austria Technologie- & Systemtechnik AG* (AT&S) is a globally operating company with headquarters in Leoben Hinterberg (Austria) which produces printed circuit boards (PCBs) and integrated circuit substrates (ICSs) for many areas of modern life in applications like mobile phones, computers, cars, medical devices and satellites. Plants are not only operated in Austria, but also in China, India, Malaysia (under construction) and South Korea, which have been built at different points in time and were subject to various regulations in those countries. This means that even though the products and wastewater (WW) streams are similar in the plants, the found solutions for WW treatment vary from plant to plant.

The most important metal that's used in PCBs and ICSs production is copper, which is laminated/deposited on an insulating layer in a way that forms conducting tracks. The structuring of the conducting tracks is a complex process with several steps in changing order, i.e. photolithography, lamination, chemical bath deposition, drilling, solder mask application, testing, and wet-chemical cleaning steps in between. A heating and/or pressing process is used to join the insulating and conducting layers together. This alternating sandwich-like stack-up of layers can be repeated as often as necessary for the specific product requirements. These production processes are the origin of WW with dissolved copper as copper complexes, CuCl or CuSO_4 .

Of course, the production of AT&S products has several environmentally important effects, such as emitted green house gases, used water, chemicals and other raw materials. AT&S is trying to reduce the impact it has on the environment and therefore has different initiatives to do so, i.e. in-house copper recycling.

1.2 Problem definition

In Leoben copper-containing WW was dehydrated and sold, but in 2018 sustainability ambitions led to the Aeris (lat. ore, copper, bronze) project, when the WW facilities were reaching their limits and an investment decision had to be made. The goals of the project were to recycle copper and chemicals while reducing overall costs, supply chain dependency, greenhouse gas emissions and waste.

The Aeris treatment consists of the collection of copper-containing WW streams, which are treated in ways that make them usable in an electro-winning process to gain reusable, metallic copper. The used treatment methods led to several patents and new WW treatment facilities in early 2023.

Since this recycling process was implemented successfully in Leoben, there have been efforts to investigate how well it would fit the new plant in Kulim (Malaysia). So far this analysis has been conducted with Microsoft Excel, estimations from experienced colleagues and companies specialized on Life Cycle Assessment (LCA). This procedure has been found to be complicated in the case of necessary adjustments, which makes it slow and difficult to coordinate between several involved departments and companies.

With this thesis and the developed simulation framework further roll-outs of Aeris (or similar adaptations) in other plants shall be simplified, become less time consuming, less prone to errors and overall cheaper.

1.3 Objectives

Necessary steps to reach this goal are to define the requirements for the software, then choose and implement a chemical process simulation software in order to build a process model of Aeris. This model is then generalized to create a simulation framework for future investigations of the applicability of Aeris.

Figure 1.1 summarizes the working methodology for the creation of this thesis. First,

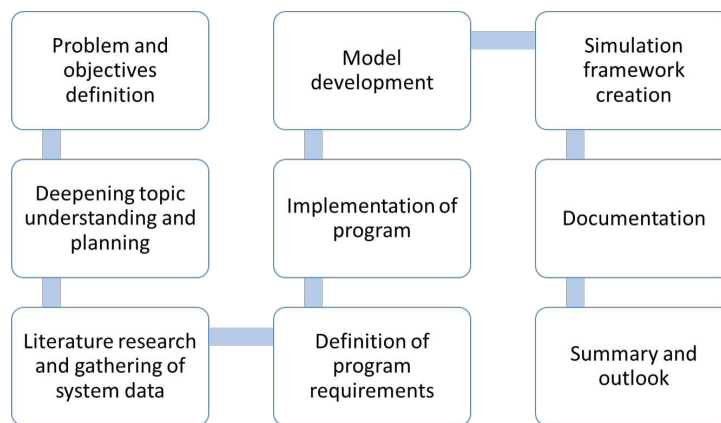


Figure 1.1: Working Methodology

the problems and objectives were defined and the understanding of the topics deepened in a way, that allowed the planning of the necessary steps. After the literature research and gathering of system data, the requirements of the simulation program were defined. A fitting program was found and then implemented in AT&S. The development of the model, validation and creation of the simulation framework were documented. Finally, a summary and outlook closes this thesis.

The structure of the thesis roughly mirrors the methodology: The introduction, problems, and objectives are presented in chapter 1. The contents of chapter 2 are the results of research in the literature, covering the topics of copper supply, wastewater treatment and process simulation. Chapter 3 documents the search for a program and the necessary steps to build a process model and simulation framework. In the end, chapter 4 summarizes the results and gives an outlook.

1.4 Project management

This short section is about the project management, which is closely intertwined with the content creation of the thesis.

It took 18 months in part-time from the original idea for this project from July 2022 until the completion of the simulation model and submission of the thesis. Especially in the beginning, the objective of the project changed several times, until everyone was sure that the found objective was the most impactful one possible.

In total, roughly three quarters of the 18 months were spent on AT&S internal organization, like finding a sponsor and deciding who should be involved in which role, but also working on security questions due to the newly required simulation software. The time for content creation itself (collecting data, deciding on a software, building the model and a simulation framework) and writing was about five full-time months, which were split-up into several intervals.

The most important aspect of project management in this project was time management: Seemingly enough time was scheduled for each milestone, but unforeseen events endangered the success of the project, i.e. project team members not being available and IT processes. To plan some back-up time and keeping a certain flexibility were therefore keys for a successful project closure. To define and maintain the status of the project, targets and milestones were used and reviewed regularly for project update meetings, where all interested parties were kept up to date.

2 Theoretical background

2.1 Copper, wastewater and its treatment

2.1.1 Economical, ecological and social considerations of copper supply

Copper is used in various industries and applications, most importantly electronics and communications, which makes it a very important metal with an increasing demand, due to its chemical and physical properties [1, 2]. The major copper trade products are concentrates, blister and anode, cathode and ingots, scrap and semis, which are shipped worldwide [2].

According to [3], copper was the third-most produced mineral raw material of a non-ferrous metal worldwide in 2021 with 21 mio. t after Bauxit with 380 mio. t and Aluminium with 68 mio. t. The biggest share of this copper was produced in Chile (26%), followed by Peru (11%), Congo D.R. (9%), China (9%) and the United States (6%). The copper market is only moderately concentrated with 57 copper-producing countries, reflected by the Herfindahl-Hirschman Index for copper of 1097 out of a possible value of $(100\%)^2 = 10,000$ for a monopolistic market. Anyhow, the U.S. Department of Energy decided to move copper from *noncritical* to *near critical* material in their latest assessment, due to the importance in electrification and growing demand [4].

Figure 2.1 shows how the worldwide copper production increased in recent years - with a growth of 33% over the course of 11 years [3, 5, 6]. Compared to 2001 with 13 mio. t [7] the production will soon have doubled, which is in line with the suggestion, that the production will approximately double every 30 years [1]. A study found that yet undiscovered copper resources will at least match the global demand for primary copper until 2050 and will add to the already identified resources. However, the exploration of new deposits will be more expensive, due to the greater difficulty of the mining [1].

The copper price is determined by producers and consumers at the commodity exchanges in London, New York and Shanghai separately for every trading day [2]. Figure 2.2 shows

historic prices of the past 60 years, in which prices fluctuated strongly and were declining towards 2000, but have quadrupled since then and surpassed mid-60s peaks [2].

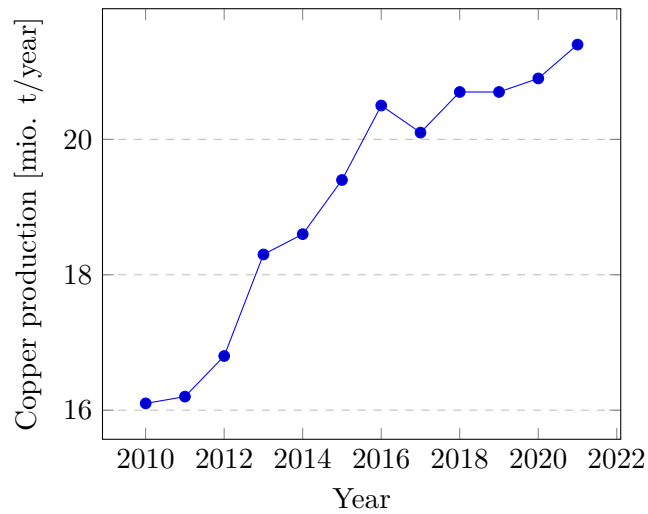


Figure 2.1: Development of the Worldwide Yearly Copper Production [3, 5, 6]

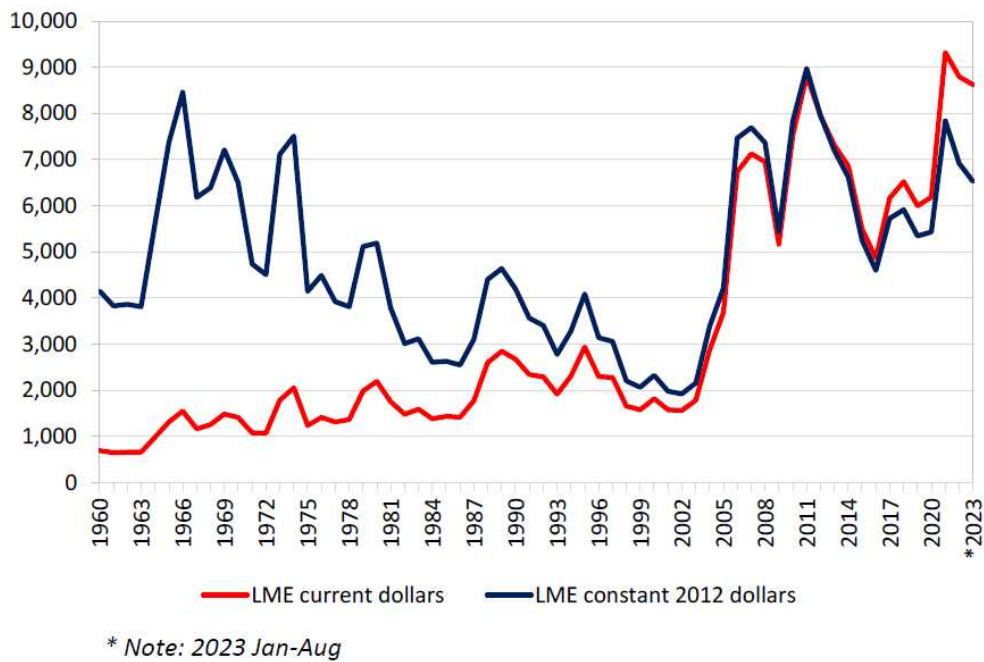


Figure 2.2: Average annual copper prices from 1960 to 2023 in US\$ per tonne [8]

The International Copper Study Group [2] summarized worldwide copper recycling: Because refined copper does not degrade or lose its physical and chemical properties, it makes the existing, circulating copper a significant copper reserve. Additionally the increased awareness for sustainability and circular economy led to an increased recycling rate of copper. In 2021 the estimated recycling rate was 33%. Even though some countries are very dependent on secondary copper, it's not enough to cover the demand and substitute primary copper completely.

Important operational and financial constraints, that can prevent copper mining are - among others - declining ore grades, bad water supply in dry mining districts, strained relationships with indigenous populations, unskilled labor markets and political risks [2].

Looking at the data and these developments it's visible that prices and production volume have been increasing simultaneously for the past 20 years, which indicates the importance of copper worldwide. Since copper is the most important metal for electronics industry it's a financially attractive choice to invest in an in-house recycling of copper.

2.1.2 Industrial wastewater

Depending on the industry, products and processes the accumulating WW is a mixture of various contaminants and pollutants and the WW flows can vary strongly, which leads to individual treatment requirements and solutions [9, 10].

Sperling [10] and Silva et al. [11] wrote the following about WW: In order to treat WW successfully, information about the total volume, number of streams and patterns of discharge must be available. On the one hand, it is usually not necessary to know the exact compounds in domestic WW, because physical, biological and chemical parameters, like the biochemical oxygen demand, are used to determine the treatment. On the other hand, metals as pollutants are more likely in industrial WW and require special care regarding toxicity and the inhibition of microorganisms.

Manufacturing of PCBs and ICs requires heavy metals, such as copper and iron, in

large quantities and other metals (nickel, gold, palladium and silver). The recyclable WW streams are metal-salt solutions originating from etching, plating and rinsing processes [12].

The term of "heavy metals" is inconsistently defined over the scientific community and therefore often misused, but for example copper is usually considered one of them, because its toxicity and density [13]. Its toxicity makes treatment mandatory and vital for every body of water that it may be discharged to [10, 11]. Although copper and many other metals are considered priority pollutants in trace amounts, they are also micronutrients, which means essential for living organisms, so their concentrations must be thoroughly controlled [14].

In addition to the concerns for living organisms mentioned and the advantages in money saving, other important aspects of copper recovery in the contemporary electronics industry are to reduce carbon emissions, secure resources, minimize water pollution and other environmental benefits [15].

State-of-the-art of copper-containing wastewater treatment

There have been conducted several reviews, i.e. [16, 17], about treatment methods for copper-containing industrial WW in the past. Even more specifically, the utilisation of WW from electroplating processes has been subject to two publications in 2022, which are briefly summarized below.

In their review Kamar et al. [18] describe several processes and provide strengths and weaknesses of them, namely coagulation and flocculation, electrocoagulation, chemical precipitation, oxidation process, bio-recovery, adsorption, membrane filtration and ion exchange. Of these, the Aeris process employs the last three methods. The combination of some of the mentioned methods has shown higher efficiencies in the removal of contaminants than single methods. Depending on the pollutants the best available combination may vary. This behavior is represented by the price: The most expensive method of removing heavy metals is adsorption alone, which costs around $4,45 \text{ \$ } m^{-3}$, and the

cheapest is adsorption with a following electrowinning process, which costs $0,35 \text{ \$ } m^{-3}$.

In a review article about obstacles and solutions of electroplating WW utilization [19] an interesting phenomenon is described: The measured values and the efficiency were significantly lower than the theoretically expected values. Reasons for this are the multiple additives, which are needed in the electroplating process. Problems and pretreatment methods for the removal of heavy metals are presented. They summarize that the combination of contaminant removal and recycling of water and heavy metal is promising.

These publications are younger than the Aeris process and confirm, what valuable impact the right combinations of methods can have on the recycling of electroplating WW. Furthermore, Aeris not only enables the treatment of electroplating WW, but all copper-containing WW, which accumulate during the production of PCBs and ICSs. The following sub-chapter will present the Aeris process and describe all the necessary methods to recycle water, HCl and copper successfully.

2.1.3 Wastewater treatment and recycling in AT&S

The Aeris project was started in 2019 in order to increase the capacities for WW treatment in AT&S, recycle copper, reduce waste, emissions and the amount of treatment chemicals [20, 21]. Metal salt-containing WW was considered a waste product with high disposal effort, but it has been shown to be economically reasonable to maintain an internal material cycle [12].

The internal calculations presented in [20] took into account all financial aspects: On the one hand the in-house wastewater treatment and recycling of copper led to cost savings for copper-clippings, chemicals, transport and external treatment costs. On the other hand, the investment for the new facilities and the operational costs e.g. for energy, staff and maintenance had to be considered. The overall result of this cost calculation was positive with a payback period of about seven years.

During the development and implementation of the recycling plant, several patents have

been filed in order to ensure a potential advantage in the electronics industry and protect the gathered knowledge. Some patents cover single process steps and others the whole Aeris plant.

The WW streams, that are treated in the Aeris process, are streams with

- high CuCl_2 -concentration,
- high CuSO_4 -concentration and
- low CuSO_4 -concentration,
- low $\text{CuC}_4\text{H}_4\text{O}_6$ -concentration.

To reuse copper in PCB and ICS production, it needs to be recovered with a purity of over 99.98%, but the WW streams named above are not directly suitable for an electrowinning (EW) process due to high concentrations of acid, unwanted metals and organic contaminants. Iron does not plate on the cathode of the EW, but reduces the efficiency of the cell, while molybdenum and nickel do plate and hinder the required high quality [12]. Additional benefits of the Aeris process is the recycling of HCl, water and the continuous recovery and reuse of H_2SO_4 within Aeris.

The goal of the WW treatment is to get an as pure as possible CuSO_4 solution, that can be plated with EW. Figure 2.3 shows a simplified flowchart of the cycle of copper, H_2SO_4 and HCl. The $\text{CuC}_4\text{H}_4\text{O}_6$ and low concentrated CuSO_4 WW streams from production are directly collected in dilution tanks, while the CuCl_2 WW streams are first passed through an acid dialysis before being added to the dilution tanks. In each of the dilution tanks water is added and the pH-value is adjusted. After the ion exchangers all treated streams are mixed and used in the EW. To lower the copper content in the discharge and therefore increase the yield, the electrolyte is transported back to the ion exchangers for a few cycles. The resulting metallic copper plates are then stripped, clipped and reused in production or sold, while the discharge is treated in a standard WW treatment facility.

The individual process steps shown in the flowchart will be explained in detail in the remainder of this sub-chapter.

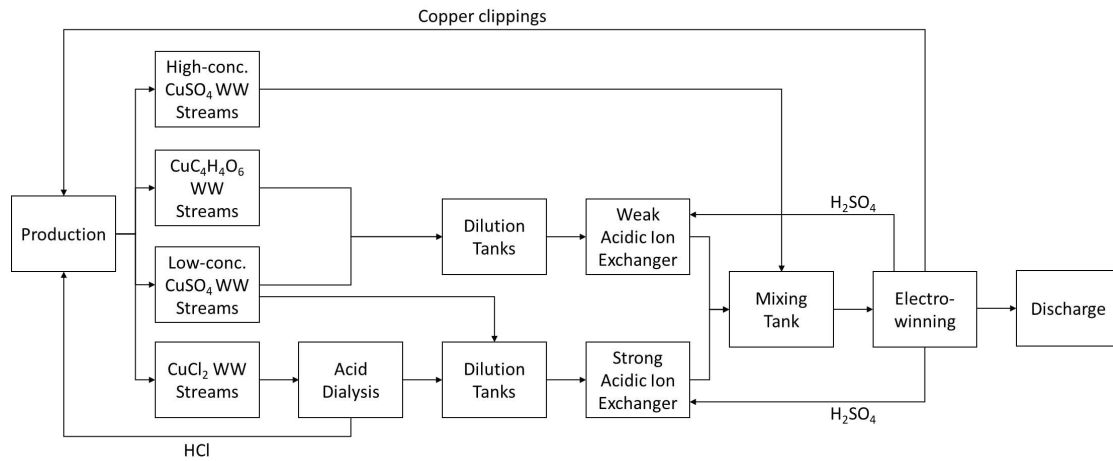


Figure 2.3: Simplified flowchart of the recycling process for copper, H_2SO_4 and HCl

Acid dialysis

Preliminary, particle filters remove particles from the WW to prevent clogging of the membrane inside the dialysis module. The acid dialysis is an essential process step, because a high content of Cl^- ions in the solution could form poisonous chlorine gas (Cl_2) later during the EW process, which causes extremely strong corrosion, or co-deposits on the electrode and reduces the copper purity. In addition, it recovers HCl , which is an important chemical for PCB and ICS production.

Acid dialysis is a concentration-driven membrane process, where Cl^- anions can pass through the positively charged membrane, while H^+ cations are held back by the membrane (formula 2.1). The reaction is improved by the continuous removal of Cl^- anions through the membrane.



The recovered HCl solution is reused in the etching process in production, which covers about 50% of the demand. The remaining CuCl_2 solutions are processed further.

Dilution tanks

These tanks are used to mix and dilute the solution with rinse/purified water, which increases the pH value and with it the retention capacity of the ion exchangers in the next step.

Ion exchangers

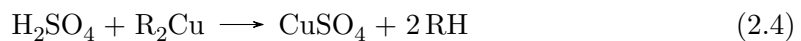
Several ion exchangers are used to separate the solution into WW with discharge quality and adsorbed copper ions in the resin to produce CuSO_4 . The strong acidic exchanger can handle solutions with a $\text{pH} > 1$. The weak acidic ion exchanger requires a pH-value over 2, which is reached by addition of NaOH (Formula 2.2):



Formula 2.3 shows how the resin (R) and copper react:



After the resin is loaded with copper it's regenerated with the copper-depleted electrolyte from the electrowinning process. Regeneration means desorbing the copper from the resin, using sulfuric acid (formula 2.4). If the electrolyte is not acidic enough, some 96% H_2SO_4 may be added.



In order to reduce the copper content of the discharged WW, two different kinds of series of ion exchangers are used, either with strong acidic or weak acidic resin. The strong acidic ones are less selective but have an increased adsorption capacity, the weak acidic ones are used to adsorb residual amounts of copper.

Mixing tank

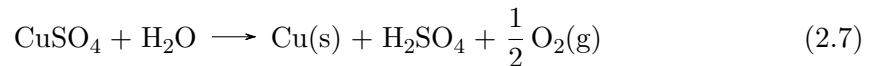
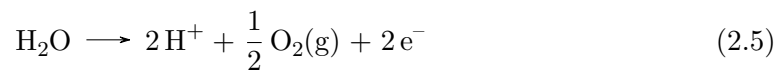
The WW stream from galvanic processes has a high copper concentration of around 50 g Cu L^{-1} and can therefore be used for electrowinning directly with only an organic

adjustment, which is done through an activated carbon filter. This stream and the ones coming from the ion exchangers are then mixed.

Because Fe could prohibit the copper deposition, the most relevant concentrations are measured continuously by UV spectroscopy for Cu^{2+} and Fe and titration for H_2SO_4 . If the Fe concentration gets too high, it's removed by a separate ion exchanger, which regenerated with water and HCl. To further ensure the electrolyte quality, a constant concentration and temperature, the tank and EW cell are equipped with a heating unit and an evaporator. In addition, there are weekly controls for Cl^- and impurities, such as nickel and manganese.

Electrowinning

Finally, the CuSO_4 -electrolyte is used in the electrowinning process. During this process, the hydrolysis of water at the anode (formula 2.5) and the deposition of copper at the cathode (formula 2.6) take place. Formula 2.7 shows the overall reaction. The EW is operated as a batch process with an average copper plating amount of $0,5 \text{ g Cu L}^{-1}\text{h}^{-1}$.



To increase the yield of the Aeris process, the copper-depleted electrolyte is used to regenerate the ion exchange resin, so its again enriched with copper. Thanks to this circulation, no or only little amount of fresh H_2SO_4 needs to be added and less water is used in the whole process.

A partial discharge of the depleted electrolyte is done to reduce eventually accumulating trace amounts of heavy metals (under 100ppm), like manganese, molybdenum or lead. This discharged WW has a low enough copper content to be treated with low costs.

Discharge

After EW the electrolyte contains copper in such a low concentration ($<5 \text{ mg Cu L}^{-1}$), that further treatment to reduce the copper content is no longer feasible with an acceptable technical effort. By adding a base, the highly acidic discharge can be neutralized cost-efficiently.

2.2 Process models and simulations

Process simulation was born in the 1960s, when hardware and software became sophisticated enough to handle complex correlations [22]. Even though, the principle of simulation is quite old, it doesn't mean that simulations are always good, because a simulation is always highly dependent on the quality of the model and data in the background [22]. An important advancement for chemical process simulation is, that nowadays most programs include a chemistry data base, basic physics and thermodynamics [22].

2.2.1 Important definitions and explanations

The following definitions of vocabulary and distinctions are most important to understand what's been done in this thesis and to avoid common misuse of terms like "model" and "simulation" [23]:

- **System:** A real process, which is the basis of the model and simulation.
- **Modeling:** The process of building a model, which represents a system.
- **Model:** A similar, but simpler, mathematical representation of a system. It should be a close approximation and include essential features, but not be too complicated. A balance between simplicity and accuracy has to be found.
- **Model validation:** A model is simulated with known input conditions and its output is compared to the system output.
- **Simulation:** Using the model of a system to experiment with different settings and study the behaviour over long periods of time, which would be hard or impossible to do with the system.
- **Simulation program:** A software, which helps to develop a mathematical model of a system, without deep understanding of programming. Nevertheless human decision making about model development, level of accuracy, test design and conclusions is indispensable.

- **Simulation framework:** A simulation framework is an abstraction of the model, which should be relatively easy to understand and/or extend, and enables multiple use cases of models, at varying levels of accuracy, to be studied [24].

In general, process simulation is the work of building a model of chemical, physical, thermal and biological processes and unit operations, which make a system, and using it for simulations [25]. These simulations are valuable for planning, training, operational management, decreasing chances of failure, avoiding unexpected obstacles, improving the processes and use of resources and many more applications [23, 25]. A good process simulation can have a big impact on cost reduction, because the best process design and properties can be found by simulation rather than experimenting [22].

The quality of any simulation depends on the accurate representation of the system, including thermal, physical and chemical properties [22]. Poor or unavailable data, wrong model parameters and over-simplification are common mistakes and can lead to severe consequences and misinterpretations [22].

If simulation is used to scale-up a system, it's important to be aware, that systems with solids are relatively sensitive and simulations may only be valid for 1:10 scale-ups, while pure fluid systems can be scaled up to 1:1000 without any problems [22]. Systems with solid components are more complex, because processes like deposition are dependent on the scale [22].

Mathematical model classifications differentiate between deterministic (input and output variables are fixed) or stochastic (input and/or output variables are probabilistic) and static (time independent) or dynamic (time dependent) models [23].

With Industry 4.0 bringing smart, interconnected systems to the forefront of modern industry standards, so called "digital twins" have become important [26]. These digital twins are the digital versions of real, physical systems, which are connected and updated in real time. This is where the differences to a model become apparent: a model doesn't necessarily represent a physical system, as it can also be used for planning and testing, and it is not updated in real time. It is of interest, though, to use recent data for a higher

level of accuracy. The purposes of digital twins are more of a monitoring, optimization and maintenance kind of nature, whereas models are rather for planning and studying systems [23, 26].

2.2.2 Model verification, validation, credibility and usability

The aspects of model verification, validation, credibility and usability should be respected in order to successfully build a useful model, that adds value to the company or project. Sargent [27] presented a tutorial on model verification and validation:

The model verification is the correctness of the model and implementation, and the validation ensures, that the model accuracy is satisfactory within its domain. The credibility of a model aims for the confidence of (future) users to use a model the trust in the derived information, while usability describes the easiness to use the model by given instructions. The verification and validation are incremental parts of the model development and should be considered during the whole process.

Like mentioned before, a model should only be as complicated as necessary, but as easy as possible. The validity of a model is based on the ability of the model to answer raised questions and the acceptable range of accuracy is defined by the output of interest. To prove the validity of a model in a certain domain and specific conditions does not mean that the model is valid all the time. The (range of) validity has to be tested and evaluated until the necessary confidence of the model is reached.

There are three approaches for decision-making if a model is valid. The first one is, that the developer decides due to the tests, which are made during development, if the model is valid or not. Another option is to let the users of the model decide about the validity, which is feasible for small developer teams. This approach also helps to increase the credibility, but a heavy involvement of the users is required. The third way is, to use a third party (no developers, users or sponsors), which makes sense for large-scale models, that involve a lot of people.

The validation should take place during the development of the model. If the model validity is not satisfying at some point, problems should be solved right away before continuing with the model development. To simultaneously increase the credibility of the model, also these steps and measures should be documented.

3 Model building and simulation

This chapter represents the practical part of this thesis and will explain all steps and problems of the process of building a model of a not yet existing system and creating a simulation framework from it. These aims require a lot of information about the processes themselves as well as the properties. Figure 3.1 depicts all steps, that are necessary to create a simulation framework, in a systematic way, starting from gathering system design and data, over software selection, model building, to a verified model and a usable simulation framework.

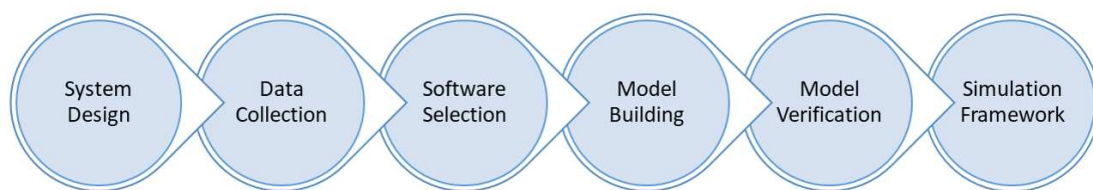


Figure 3.1: Necessary process steps to create a simulation framework

Going down further in detail the part of building a model covers several steps, which will represent one sub-chapter each [23, 28]:

1. Identifying and formulating of problems,
2. collecting and processing of system data,
3. comparing and selecting of software,
4. formulating and developing the model,
5. validating the model,
6. creating the simulation framework and
7. documenting for future use.

3.1 Identification and formulation of problems

The first step is to identify current problems and defining them, in order to make them approachable.

As briefly mentioned in the problem definition (chapter 1), the Aeris system has been designed and implemented in the Hinterberg plant (Austria). There have been efforts to analyze the potential of making the system usable in other plants of AT&S - especially the new plant in Kulim (Malaysia) - and to be able to sell the system on a licence basis to external customers, i.e. PCB manufacturers. These efforts were driven by some of the Aeris engineers, newly involved people and external consultants. This "manual" analysis has been slow, inefficient and prone to errors, which is why the decision was made to improve this process in the future with the aid of a simulation framework.

Therefore, the main goal is not to improve the Aeris system itself, but to increase agility and cost-effectiveness in future projects of Aeris implementations in other plants or investigations into possible process adaptations by using the simulation framework.

From the setup of the Aeris plant and the provided data, the needs were defined to be addressed by a mathematical, deterministic and dynamic model (theory in chapter 2.2). The search for a software was therefore based on these properties.

3.2 Collection and processing of system data

The new plants in Kulim are still under construction and therefore only estimated data is available yet. However, the advantage of PCB and ICS productions is, that WWs from different PCB plants are very comparable, because the production processes are similar - the same is valid for ICS WWs.

This advantage was the key for the estimation of the data for Kulim: The accumulating WWs of existing and running plants are very well known and represent a good reference for such estimations. The data for Kulim was already consolidated before this thesis

started, because it was needed for a LCA study beforehand. The estimation was done by experienced engineers with deep knowledge of the existing plants and the plans for the new ones in Kulim. For that reason, it is assumed that the provided data is of good enough quality to be used for the model. In addition to that, the model is adjustable anytime, and any surfacing errors can be easily corrected.

Following information have been provided for all relevant streams in Kulim plants:

- total number of WW streams
- production and process origin
- copper compound
- copper concentration
- batch volume
- constant overflow volume
- number of machines
- number of services (batch discharges) per year

All this information can be found in the appendix (chapter 6) in tables 6.1 and 6.2.

Additionally, information about batch sizes, chemical reactions and process duration has been gathered from the Aeris engineers along with the verification process.

3.3 Comparison and selection of software

To use a simulation program has advantages such as reduced knowledge requirements, user guides, user interface, animations, flexibility and automatic collection of statistics [23]. The increasing number of simulation programs available means, that most have specific fields of applications, which they are intended for [25]. Even though most might be usable for originally not intended use cases, it makes sense to choose a program that is specifically made to fit a certain kind of system and problem [25].

The process of making a decision about which simulation software to use is complicated, because the building of system understanding is necessary first, in order to be able to consider all relevant properties of the software. To achieve this knowledge and understanding, conversations with colleagues, visits to the plant and collecting the most important features are key activities.

In general, a decision matrix is used to analyze requirements and the fulfillments of those by several possible solutions in a systematic way. The requirements are weighted according to their importance and the options are graded from zero (no fulfillment) to five (maximum fulfillment). The scoring is then multiplied with the weighting and all resulting weighted scorings are summed up for each option. The options are then ranked from the highest to the lowest overall sum, which means the highest rank represents the best fit.

The software had to be able to depict several copper-containing WW streams with volume and copper content, and consider the dynamics of the production, meaning the discontinuity of batch processes and continuity of overflows. An online research was conducted to collect a list of available dynamic, chemical process simulators. This list was then shortened by filtering them by the above features. The remaining softwares were then combined with the additional criteria below to fill out a decision matrix, and structure the evaluation and selection of a simulation software out of the available options. These following requirements were defined in order to find the best-suited simulation software:

1. Software Costs in budget
2. Calculation of environmental footprint
3. Calculation of operational costs
4. Calculation of energy demand
5. Quality of graphical interface
6. Overall user-friendliness

In detail, five dynamic, chemical process simulation softwares have been looked into: Aspen Plus [29], AVEVA [30], DWSIM [31], ITHACA [32] and SuperPro Designer [33].

Table 3.1 shows the decision matrix, which summarizes all the requirements with their weightings, the considered softwares with their (weighted) scorings, the resulting sums and ranking.

As an example for the whole scoring process and filling out of the decision matrix, the scoring of the software costs is explained: The yearly license prices of Aspen Plus (30.000\$/year), AVEVA (7.000\$/year) and SuperPro Designer (7.000\$/year) are out of the budget and therefore got a scoring of zero, while DWSIM is a open-source freeware, which resulted in a scoring of 5, and ITHACA (1.000\$/year) is comparatively cheap, getting a score of 4.

The scoring of the other requirements was more difficult, because they are subjective. For some of the softwares (AVEVA, DWSIM and ITHACA), free trial versions were available and could therefore be tested by following beginner guides or video tutorials. Aspen Plus and SuperPro Designer could not be tested personally, but were scored by watching online video tutorials and their appearance on the websites ([29, 33]).

Table 3.1: Decision Matrix for Software Selection - Weighting (W.), Scoring (S.), Weighted Scoring (W.S.)

		Aspen		AVEVA		DWSIM		ITHACA		SuperPro	
Requirement	W.	S.	W. S.	S.	W. S.	S.	W. S.	S.	W. S.	S.	W. S.
Softw. Costs	20%	0	0	0	0	5	1	4	0,8	0	0
Envir. Calc.	5%	3	0,15	5	0,25	0	0	0	0	5	0,25
Cost Calc.	5%	3	0,15	0	0	3	0,15	0	0	5	0,25
Energy Calc.	5%	5	0,25	0	0	5	0,25	0	0	5	0,25
Interface	25%	5	1,25	5	1,25	5	1,25	5	1,25	4	1
User Friendl.	40%	5	2	3	1,2	3	1,2	5	2	5	2
Sum	100%	3,8		2,7		3,85		4,05		3,75	
Rank		3		5		2		1		4	

A decision matrix is a good tool to get an overview of requirements and their fulfillment, but it's important to notice that the results can be easily changed by an adjustment of weighting or underlying decisions and therefore result may vary. Looking at the fulfillments, other than software costs, it appears that Aspen Plus or SuperPro Designer would have been a better fit, if the budget was higher. The question of increasing the software budget might arise, but the budget was defined in a way, that justifies the software costs by compensating for them with a potential reduction of working hours in the future. For this reason, the results of a decision matrix are helpful, but should be regarded with care.

The process of finding the right simulation software for the given application and future use in the company was a time-consuming, complicated, iterative one. In the end, several fitting softwares were found and some tested, which led to the final decision for ITHACA, which was then implemented in AT&S after going through an internal approval process, including security and compliance checks.

3.4 Model development with ITHACA

In this sub-chapter ITHACA and model building in ITHACA are described and all the following information refers to the program itself [32] or the user manual [34]. The flow sheet of the model can be found in the appendix in figures 6.1 and 6.2.

ITHACA is a publicly available, dynamic, chemical process simulator, in which every process is built from a basic block, called ITHACA Process Unit (IPU). A process can be configured to match physical and chemical parameters, and be saved to a library for sharing and reuse. In order to match real process behaviour, process control and logic can be configured and visualized for every IPU. In total nine properties can be set by the user, which are: name, description, total volume, overflow volume, operating pressure, operating temperature, input heat, input work and status.

The data visualisation widgets can display parameter values and calculation results.

Between IPUs, mass and energy flow information can be specified and transferred. Additionally, events, like batch discharges and down times, can be configured. Any occurring chemicals, phases and components must be defined beforehand and can be used for chemical reactions in the IPU settings. The only feature that isn't used in this model, is the stochastic value generator, which can be used to assess risks, i.e. equipment break-downs.

Every element in ITHACA gets its own unique ID number, by which it can be referred to, and every kind of element starts from "1". So while there may be several elements with the ID number "1", it can never be the same kind, i.e. IPU 1, stream 1, splitter 1. During simulation Microsoft Excel files are saved containing all calculated data about IPUs and streams (masses, volumes, densities, flows etc.).

3.4.1 Adding phases, components and reactions

First, all phases and components, which should be represented by the model, are added to a database (figure 3.2). The relevant names, chemical formulas and density data can be found in table 5.4. In this case all defined phases and components are needed in the model, so all boxes are checked to make them available in the model.

The data for all WW streams can be found in the tables 6.2 and 6.1. Since only the mass concentration of copper is given, the molar concentrations are calculated by dividing the mass concentration by the molar mass of copper. Using the 1:1 stoichiometry of the copper cations to the corresponding anions in the solutions of CuSO_4 , CuCl_2 or $\text{CuC}_4\text{H}_6\text{O}_6$, the molar concentrations of the dissolved compounds are the same as the molar concentration of the copper. Formula 3.1 shows the calculations exemplary for the calculations of all WW streams. The molar concentrations are then directly used in the model.

$$c_{\text{Cu}} = \frac{\rho_{\text{Cu}}}{M_{\text{Cu}}} = \frac{18,5 \text{ g } L^{-1}}{63,55 \text{ g mol}^{-1}} = 0,29 \text{ mol } L^{-1} = c_{\text{CuSO}_4} \quad (3.1)$$

After adding a source stream to the model, the composition of the stream can be set in

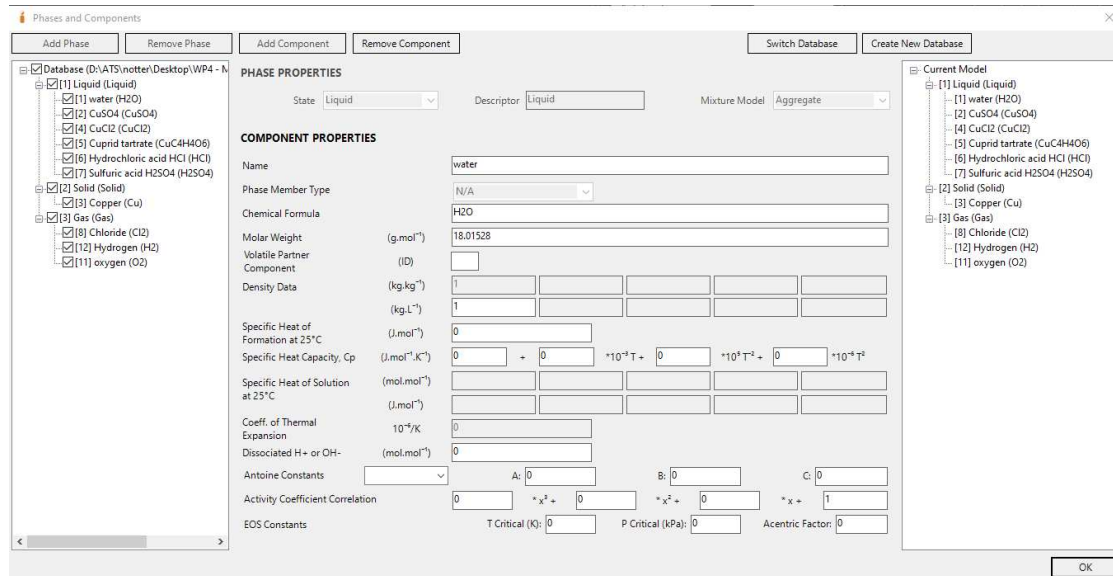


Figure 3.2: Definition of Phases and Components in ITHACA

the "Composition" tab. In figure 3.3 the exemplary calculated $0,29 \text{ mol L}^{-1}$ are set for CuSO_4 in the liquid phase, which triggers the automatic calculation of the other shown values, which were set to a value unequal to 0 before.

The screenshot shows the 'Stream 2 - Properties' dialog box, 'Composition' tab. It displays the following composition data:

ID	Name	(w/w)	(g/L)
1	Liquid (Liquid)	1	1033.4291345229
2	Solid (Solid)	0.0000000000	0.0000000000
3	Gas (Gas)	0.0000000000	0.0000000000

ID	Name	(w/w)	(g/L)	(mol/L)
1	water	0.9552107712	987.1426405681	54.7947431607
2	CuSO4	0.0447892288	46.2864939547	0.2899999997
4	CuCl2	0.0000000000	0.0000000000	0.0000000000
5	Cuprid tartrate	0.0000000000	0.0000000000	0.0000000000
6	Hydrochloric acid HCl	0.0000000000	0.0000000000	0.0000000000
7	Sulfuric acid H2SO4	0.0000000000	0.0000000000	0.0000000000

The dialog box also includes a 'CUSTOM' dropdown menu and 'Data Sources', 'Modes', 'OK', and 'Cancel' buttons.

Figure 3.3: Composition Tab in ITHACA

IPUs can be used to represent a lot of different processes, so if needed reactions can be added via the "Chemistry" tab (figure 3.4). Reactions can be added by using the previously defined components of the model. The shown reactions are dissociations of defined components in water into the corresponding ions. The conversion rate can be adjusted to fit the real process by adding a factor or a rate of disappearance. For something dissolving completely, i.e. a salt in water, this factor would be 1. Note that ITHACA has issues with factors being 1 (chapter 3.4.4).

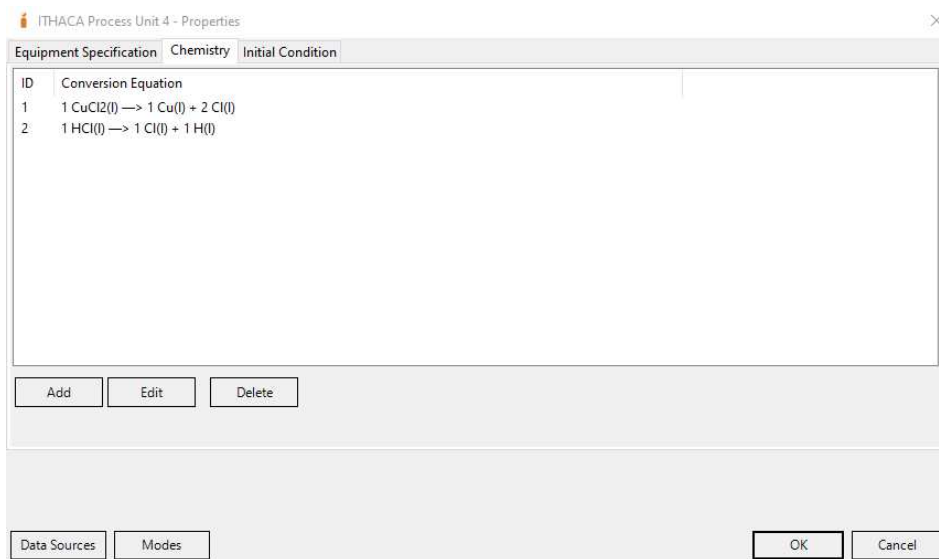


Figure 3.4: Chemistry tab in an IPU in ITHACA

3.4.2 Timing of WW streams

By clicking on the "Modes" button in any IPU an additional window opens (figure 3.5), where the flow control can be defined amongst other things. For all input WW streams in this model, "Mode 1" represents the overflow stream and "Mode 2" represents the batch emptying stream, which are then automatized by timers to switch according to the given number of services per year.

While setting the timing of the batch emptyings in ITHACA, several questions regarding the real timing arose. The provided data only stated the number of emptyings per year,

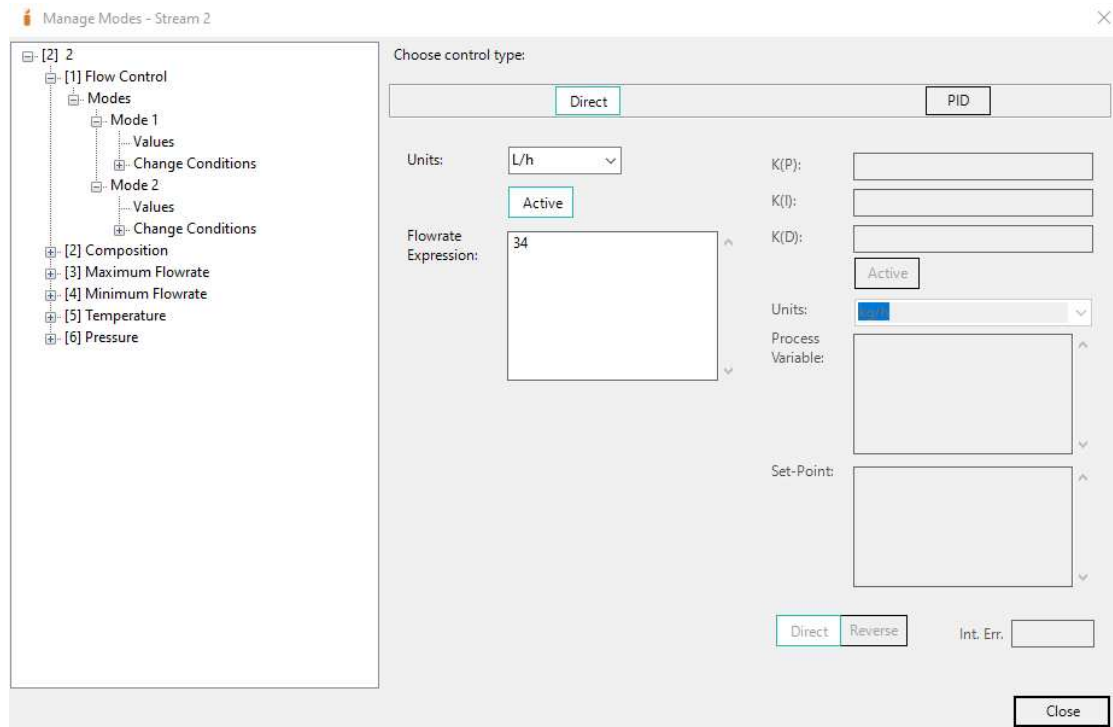


Figure 3.5: Definition of the Stream Modes in ITHACA

but no information, like duration of the procedures, regularity of the time spans in between and time-wise overlapping of different emptyings were available. After consulting a maintenance engineer it was therefore assumed, that the emptyings are periodically and that it always takes 1h to empty and refill a batch. Regarding, that most batches are smaller than 3 m^3 and are emptied often (up to 66 times a year), a fast and optimized batch renewal is important for production.

Figure 3.6 is an exemplary screenshot, in which some WW streams (2, 4 and 5), their constant overflow, inconstant batch flows and total volume in the storage tank (IPU 3) are shown. The output flow 20 in this example is set to 0, to investigate the volume input to the storage tank. Streams 2, 4 and 5 each condense several, smaller streams with the same characteristics (table 6.2).

The impact of simultaneous emptyings was investigated: For streams like 2 and 5, with

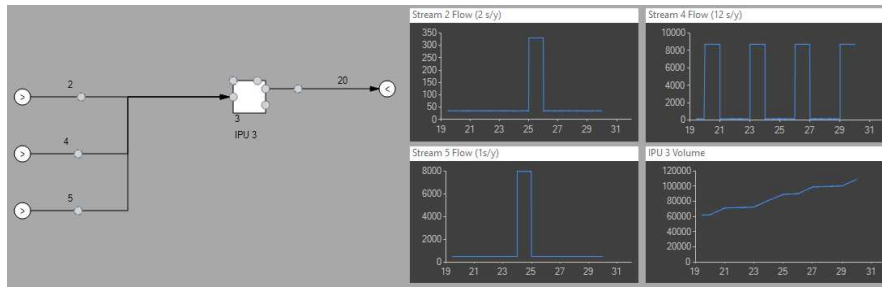


Figure 3.6: Integrating the timing to the WW streams in ITHACA (2, 4, 5...input streams; IPU 3...storage tank; 20...output stream)

only one and two emptyings per year, the emptyings only account for 0,2% of the total stream volumes per year, so the timing of these streams has little impact on the sizing of tanks. The batch emptyings in stream 4 make for 7,9% of the total volume per year, but these are split into 12 emptyings and therefore also have little impact in the overall volume development. All streams with higher percentages, than the mentioned ones (i.e. stream 13 with no constant flow at all) are emptied 36 - 66 times a year, which distributes the accumulating volume well over the whole year, into roughly weekly intervals. When dividing the batch volume by the weekly overflow volume per stream, the share of the batch emptying is between 10% and 34% for most streams, the highest value being 46%, which proves that the overflow volumes are the primary WW sources.

In the given example, all the emptyings of a years time span are conducted in 24h and the screenshot shows the end of this "compressed year". This was done to enable a quick check, if all timers worked properly. One can see how the volume development in the storage tank is an almost linear line, even though the emptyings are far closer together than they would be in reality, and the batch volumes are therefore way higher in comparison to the continuous stream volumes. Due to the combination of multiple small streams, i.e. stream 5 is coming from 14 machines in two different plants, the accumulating WW is potentially even more distributed over time, than represented by the model. All this supports the assumption, that the timing of the emptyings is justly simplified and without much impact on the accuracy of the model.

3.4.3 Adjusting concentrations and volume streams

At several points in Aeris streams are split and treated further separately, i.e. the acid dialysis. The recovered HCl-stream was estimated to be $98,2 \text{ kg h}^{-1}$ with a concentration of 10 %. Using the given volume stream and 10 % output concentration to add a controlled stream, these parameters can be met accurately, like shown in figure 3.7.

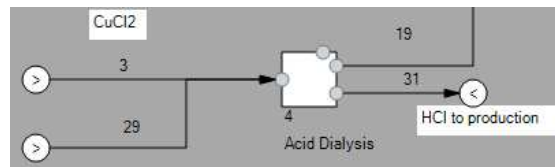


Figure 3.7: Using a controlled stream to match requirements in ITHACA (3, 29...input streams; IPU 4...acid dialysis; 19...overflow stream; 31...controlled stream)

Figure 3.8 is a ITHACA screenshot of a configured splitter: A splitter separates a stream into two streams by using factors on the incoming mass, phase or component. After selecting the split basis the properties of how much is sent into the "top stream" can be set between 0 to 1. This splitter is used after the EW to separate the outgoing stream into copper sheets and the copper-depleted stream. In this case the phases are used as a basis and all of the solid phase is separated.

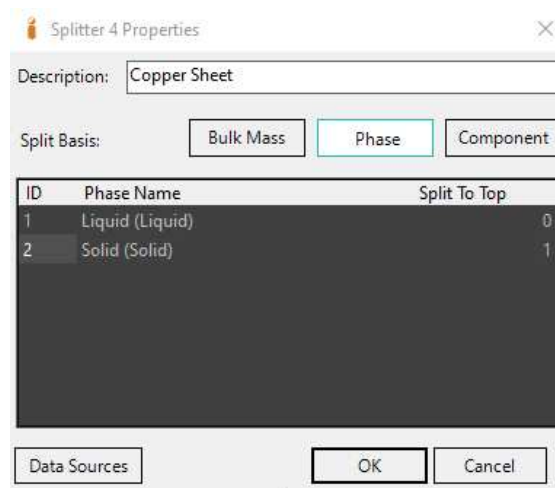


Figure 3.8: Splitter Properties

3.4.4 Limitations of the software

During the model building some problems with the software were encountered, which could be solved mostly, but should be addressed again when improvements to the software have been made. Additionally, a bug with referencing concentrations of other streams was found, which was reported, but could not be resolved in time.

The first issue was, that the solver could not handle empty streams well. For example, stream 47 was empty at the beginning of the circulation of the electrolyte. IPU 5 was supposed to split stream 47 into three streams with specific ratios, but couldn't handle a volume flow of 0 in stream 27. This was solved by adding a small 1 L of water to IPU 5 in the initial condition tab.

The second problem concerned pH values. In the real system the addition of NaOH and H₂SO₄ to the ion exchangers is handled by measuring the solutions continuously and adding the required amount of base/acid automatically. Sadly, the calculation of the pH value of mixed solutions doesn't yet work in ITHACA, which means that the automatic dosing of base/acid could not be implemented. Because of the already mentioned bug, it was not possible to match the streams in a way that equals the discharged H₂SO₄ amount. So those streams H₂SO₄ were added and set to even out the discharged volume. The NaOH was not included, because the demand is so unsteady, that there was no way to include it in an accurate way.

Thirdly, it was found, that the reaction equations slowed down the simulation speed so significantly, that a full run wasn't possible anymore. Therefore, one made simplifications was to enter the start concentrations split up into ions right away to avoid the reaction equation for the dissolving. For example, instead of 0,5 mol H₂SO₄ L⁻¹, the ion concentrations of 0,5 mol SO₄⁻² L⁻¹ and 1,0 mol H⁺ L⁻¹ were entered.

Concerning every setting with factors, it's important to understand that ITHACA uses a solver, which tries to find solutions to balance all equations with the smallest possible error. Every time there is an factor of 1 (i.e. reaction rate or stream references), this

reduces the number of possible solutions and slows down the simulation speed significantly. By sacrificing some accuracy (i.e. factor of 0,99 instead of 1), the simulation speed can be increased a lot.

Before these issues were identified, the simulation speed became so slow, that the model wasn't practical. This impacted the development of the model a lot, because changes could not be reviewed easily. Since modelling is all about finding a balance between accuracy and simplicity these issues have to be considered for each individual setting.

3.5 Model validation and verification

The theory of model validation and verification was explained in chapter 2.2.2. Like already mentioned there, the validation should take place during the model building. Two of the later users supported in the task of validation and verification during meetings, in which the progress of the model was presented and discussed.

At the start of modelling, most collected data was about the process flow and the WW streams. This data was sufficient for a first model draft, which included:

- Phases and chemical components,
- WW streams and their timings,
- process steps including chemical reactions and
- connections between processes.

The first draft served the purpose of identifying all the gaps before paying attention to further details. This way, the volumes and concentrations of all the streams in the model were made comparable to the real system, which is an important part of the model validation. For example, a too low Cl-concentration in the output stream might be due to a wrong assumption on how well the membrane of the acid dialysis works and a too high Cu-concentrations between process steps could hint to too little dilution with rinse water. Thanks to questioning and comparing the model like this, processes can be

adjusted to fit the system and real-world data.

During building the first draft several gaps in the gathered data, like details on tank sizes and process durations, became apparent as well. In the beginning, these gaps posed no problems, because it's easy to edit a tank size or process duration. In order to achieve a high level of accuracy in the final model, these gaps had to be addressed, though. In validation and verification meetings those blanks were filled and discussed with the Aeris engineers, which are also the future users of the model.

The second draft was about getting all streams, connections and dependencies right. Additionally, some simplifications were identified in the meeting, which improved the simulation speed (chapter 3.4.4). Further, a simplification regarding the EW was agreed on: Since the electrolyte is circulated over the ion exchangers, mixing tank and EW, the EW was simplified to a continuous process. The system is actually a batch process with partial copper removal ($35 \text{ to } 10 \text{ g L}^{-1}$), but thanks to the circulation finally all of the incoming copper can be plated, so this simplification was made to reduce model building and simulation time. This change doesn't affect the amount of recovered copper, but rather the mode of operation.

An issue was found with the provided data, more specifically the services per year. According to table 6.1 streams 6, 9 and 10 are emptied twice a year. During the meeting it turned out, that in fact it's rather an "on demand" procedure and the batches are only emptied partly. Therefore, those streams were evenly split up into 12 services per year.

After the implementation of all adjustments to the model another meeting took place. Remaining questions were discussed and only some small changes to the model defined, such as relations between streams. The third draft of the model was therefore determined to be the final version and the foundation for the simulation framework.

In the third version, streams, connections, splitters and IPUs were validated, and only some factors and volume streams remained to be adjusted. At this point the simulation ran without errors and worked like intended. After adjusting the discussed parameters the model was ready for verification.

For the verification, real system data, provided by the Aeris engineers, was used and compared to the simulation results for the stream of plated copper (stream 45). From the information about concentrations and volumes of all WW streams an average mass stream of copper can be calculated. The streams in table 6.1 add up to 184 kg Cu d^{-1} and the ones in table 6.2 to 822 kg Cu d^{-1} . In total, an average of $1006 \text{ kg Cu d}^{-1}$ enters the Aeris process. According to the provided data 948 kg Cu d^{-1} (94,2 %) of the incoming copper is plated and the rest is discharged at the ion exchangers (streams 39 and 44) and with the discarded electrolyte (stream 40).

From the saved result file the mass flow of plated copper can be retrieved. IPU 10 was specifically included to represent a storage. From the results file the average copper per day can be calculated. After two days of running the simulation a random check at 1.366 out of 8.000 productions hours per year provided an average of 955 kg Cu d^{-1} and therefore 94,9 % of the incoming copper. The deviation of only 7 kg Cu d^{-1} and 0,7 % means that the model is very similar to the system data and can therefore be verified and further used for the framework.

A random check at 4.861 hours, showed that the average per day of the plated copper had increased to 991 kg Cu d^{-1} and 98,5 %. In the end the average was at 996 kg Cu d^{-1} and therefore 99,0 %. This change over time is still in an acceptable range but apparently, the loses of copper in the EW cycle model are lower than those in the system. This represents a good point of investigation and for further improvement of the model by future users.

3.6 Creation of a simulation framework

The completed model can be used to simulate the system over a desired time frame with specific time steps and adjustable calculation precision. During the simulation, the progress is visualized in widgets and report charts and all results are saved into an Excel file, which allows further analysis. The ITHACA exports of the model and the simulation framework are attached in the appendix in the figures 6.1, 6.2, 6.3 and 6.4.

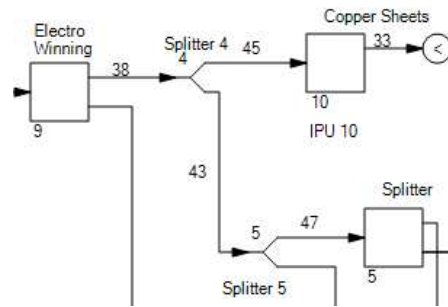


Figure 3.9: Screenshot of the electro winning process in the model in ITHACA

The point of a simulation framework is to make the model more accessible for future users, who might not have or need a deep understanding of the system itself. Through grouping of process units, splitters, streams etc. these groups become black-boxes, which means the model has less parts and becomes easier to understand. By using "expressions" for settings, the model can be easily adjusted if necessary, i.e. the size of the EW tanks or the number of production hours. Everything else, like how streams are split or conversion rates are only changeable indirectly, by selecting a group and a part of that group, which does not show the connections, but only names.

Figure 3.9 shows a screenshot of the EW process with all IPUs, splitters and streams of the model. Figure 3.10 is a screenshot of the same processes, but grouped for the simulation framework. For the framework the IPUs, splitters and streams were grouped and the usual IPU square was replaced by a ITHACA icon to represent the EW process in a nicer way. With a right click on the picture in ITHACA all the underlying process parts are accessible to change, if needed. It only shows the name of the parts and their IDs and not how the parts are connected. If the provided name is not enough to identify the parts/connections the export of the model has to be used (figures 6.1 and 6.2).

Additionally, graphics for stream volumes and concentrations are added to provide more information at a glance (figure 3.11). The figure shows how the copper concentration and amount of produced copper sheets increase in the beginning of the simulation. The mixing tank, which feeds the EW tank, and the EW tank itself are filled with an aqueous

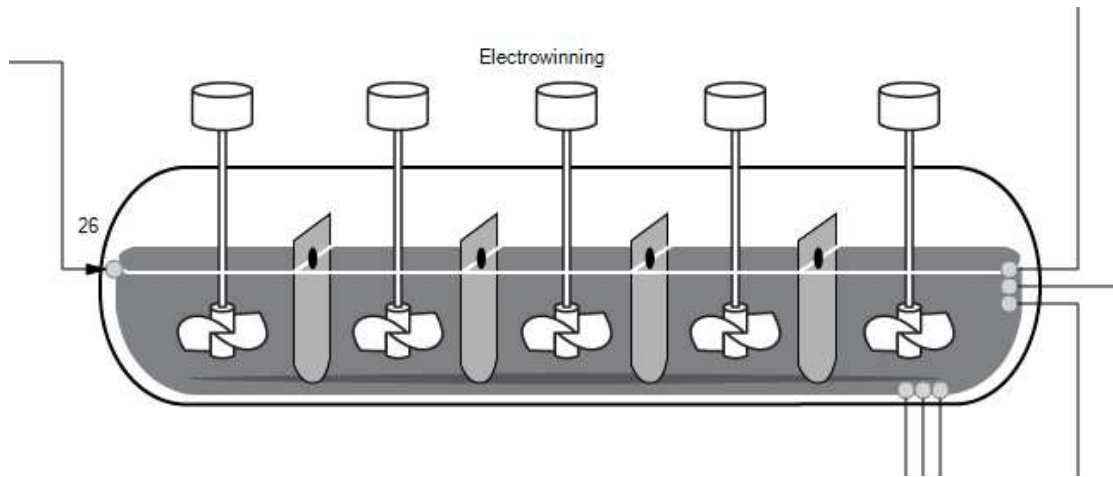


Figure 3.10: Screenshot of the electro winning process in the simulation framework in ITHACA

H_2SO_4 solution in the beginning and copper is only then brought into the system, when the WW streams start coming in.



Figure 3.11: Provided graphics depicting the copper concentration in a stream and the EW tank and the produced copper sheets in ITHACA over time in hours

With these optical improvements, grouping of process steps and graphics the simulation framework is more user-friendly than the model and provides an easier way to look into the Aeris set-up.

4 Summary, conclusion and outlook

In this chapter, the reasoning and background for this thesis will be condensed. All activities summarized, set goals revisited and compared to the achieved results. Finally, there will be an outlook on the further usage of the model and the simulation framework.

4.1 Summary

All AT&S products contain copper, which makes its supply an important factor for successful business. In the past, copper prices were volatile, but the availability was good. Recently though, copper was declared a "near critical" mineral by an U.S. department's assessment, due to rising demand over various industries on all continents. Recycling copper is a powerful way to ease the strain on the supply chain and produce more sustainably. By usage of secondary copper, the amount of primary copper can be reduced, and with it the resource intensive mining, smelting and transport thereof. To ensure a reliable, low-priced, high-quality copper supply is therefore not only meaningful for risk minimization and meeting sustainability goals within AT&S, but also on a global scale. An additional benefit of Aeris is the recycling of hydrochloric acid, which makes the facility even more effective.

The Aeris process is the state-of-the-art AT&S answer to address this topic and was ramped up in 2023 in AT&S Hinterberg. In Aeris several different copper-containing WW streams are treated, to gain secondary metallic copper through an electrowinning process. Additionally, HCl is recovered and recycled.

Because other plants don't yet have their own facilities to recycle copper, this thesis is the start of using process models and simulation to investigate further roll-outs of Aeris, more specifically the new plant in Malaysia, that's currently under construction. The first work package was gathering knowledge and data about Aeris. Secondly, choosing and implementing a fitting process simulation software company wide. In the third step

the model for Aeris was built, verified and used to provide a simulation framework for future projects.

Gathering data about existing facilities like Aeris is complicated. An advantage here was, that all process engineers, who built Aeris are still in AT&S, so in theory the knowledge about the facilities was there. The challenge in collecting data was, that the estimations for Kulim were revised many times, and often it is unclear, which version of each corresponding file is the latest one. Additionally, information is shared in various forms, like oral testaments, flow sheets, Excel files and patents.

After getting a rough picture about Aeris, a suitable software had to be picked. Before this thesis, no process simulation software had ever been used in AT&S, so several criteria were defined to compare the options data-based and to finally find the best software for this project and beyond. From a list of almost 100 available chemical process simulation softwares, five were picked to be looked into closely. Based on the criteria, ITHACA was the best-suited software and led to company wide implementation.

ITHACA provides a quick start guide with examples to work on and get to know the basic features and a user manual. Using those two files it was possible to start building the model by adding all phases, components and the incoming WW streams to the sheet, including their timers to match batch emptyings. By addition of chemical reactions and different operational modes to the processing units they can be adjusted to represent any real process. By using tools like combiners and splitters, streams can easily be handled.

During model building several issues with the provided data were encountered. Some sources of data, i.e. Excel sheets, process descriptions and flowcharts about Aeris were inconsistent or turned out to be missing. It was clear, that all information was somewhere in the company, but aligning all different kinds of sources into one up-to-date model was a process of many meetings and reviews of data.

Element Process, the company that provides ITHACA, is very small and there is still much potential for further improvements in the software. For example, there are no backup files saved automatically and there is no return button, which unnecessarily

complicates the work. Also, there were bugs found and reported but not resolved quickly enough, so other ways had to be found. If the simulation stops, due to some issue with the model, it does not say, where the problem is, so finding and resolving errors is almost impossible, if the simulation is not started after every change of the model, which again complicates working with ITHACA. The solver also has issues with empty streams and conversion rates in reactions of 100%. In the best case the simulation becomes slow, in the worst case it causes an error. To avoid these points, some simplifications and adjustments were necessary, which caused several revisions of the model, which posed a huge hazard for errors. Anyhow, it was possible to develop a satisfactory model of Aeris, which was verified with the Aeris engineers.

The developed simulation framework is a simplification of the model for future users, which enables changes to the model without the need to adjust every parameter, thanks to links between the components of the model. The appendix contains screenshots of the model and the framework (figures 6.1 - 6.4), where the groupings are visible, especially the for the EW part. Comparing them to figure 2.3, which shows the simplified flowchart, the process flow is the same. It is apparent though that there are a lot more streams, i.e. the rinse water (stream no. 11) or the iron elimination (stream no. 48). Also the EW process is divided into several steps in the model to properly include everything that's happening.

4.2 Conclusion and outlook

The objectives were to find a software and use it to build a model and a simulation framework to further help with Aeris roll-outs. These goals were met, but there are still many potential improvements.

The model could be further improved in several points: By using the "reading/writing to Excel sheets", settings in processing units could be automatized and made more user friendly by designing an input Excel sheet. This would help people, who are less experienced with process models and simulations. Once the found bugs are removed and

the potential improvements are implemented in ITHACA, it will be possible to integrate things like the automatic dosing of bases and acids in the model.

Since this was the first time anyone worked with a process simulation software in AT&S there was not much support or expertise available. When choosing the software, the costs unintentionally restricted the selection a lot. It is hard to estimate how big the impact of a higher budget would have been. With a two times higher budget a different software (SuperPro Designer) would have been chosen, and with a significantly higher budget the decision would have been different again (Aspen Plus).

On one hand, it's planned to use ITHACA, the model and the simulation framework for several projects in the future, so maybe a higher budget would have been justified. On the other hand, AT&S is new to using these kinds of tools and there is no guarantee for success and people adopting new ways of working.

By choosing a cheap software, the financial risk was minimized, but at the same time the likelihood of acceptance and usage in the future might be reduced, because of the complexity and relatively low maturity level of ITHACA. A good change management and enabling people to learn how to use process models and simulation to their advantage will be the keys to a successful continuation of ITHACA and process modeling and simulation in AT&S.

The further plans are to use the model and framework for the new plant in Kulim (Malaysia) to investigate the copper recycling from WW there and use it as part of an LCA for the site.

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5.2 List of Abbreviations

Abbreviation	Meaning
AT&S	Austria Technologie- & Systemtechnik AG
EW	electrowinning
ICS	integrated circuit substrate
IPU	ITHACA Process Unit
LCA	life cycle assessment
PCB	printed circuit board
WW	wastewater

5.3 List of Symbols

Symbol	Meaning	Unit
c	molar concentration	$mol L^{-1}$
M	molar mass	$g mol^{-1}$
ρ	mass concentration	$g L^{-1}$

5.4 List of Chemicals

Chemical Formula	Name	Density [35] $g L^{-1}$
$C_4H_6O_6$	tartaric acid	1,79
Cl^-	chloride ion	
Cl_2	chloride	
Cu^{2+}	copper ion	
Cu	copper	
$CuC_4H_4O_6$	cupric tartrate	
$CuCl_2$	copper chloride	3,39
$CuSO_4$	copper sulfate	3,60
Fe	iron	
H_2	hydrogen	
H_2O	water	1,00
H_2O_2	hydrogen peroxide	
H_2SO_4	sulfurid acid	1,84
HCl	hydrochloric acid	1,64
O_2	oxygen	
$NaOH$	sodium hydroxide	
R	resin	

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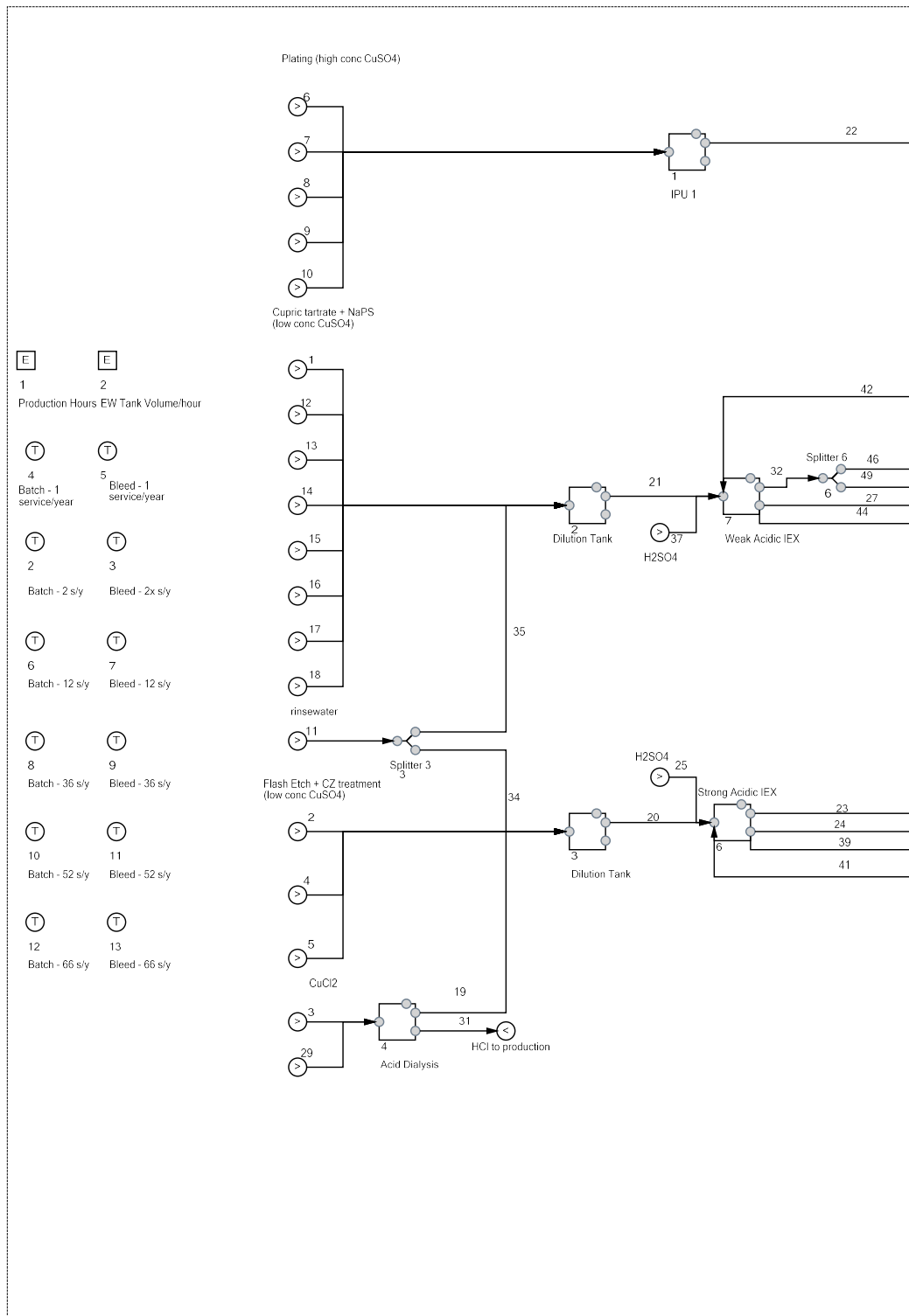
6 Appendix

Table 6.1: Information about WW streams from copper plating used for modelling

Ithaca Stream No.	Compound	Batch L	Overflow $L h^{-1}$	Concentration $g L^{-1}$	Services No. per year	Machines No.
6	CuSO ₄	2000	0	56,0	2	8
6	CuSO ₄	2000	0	56,0	2	1
6	CuSO ₄	2000	0	56,0	2	9
6	CuSO ₄	2000	0	56,0	2	2
7	CuSO ₄	6000	4,5	63,0	1	1
7	CuSO ₄	6000	4,5	63,0	1	1
7	CuSO ₄	6000	4,5	63,0	1	1
7	CuSO ₄	6000	4,5	63,0	1	1
8	CuSO ₄	6000	4,5	66,0	1	1
8	CuSO ₄	6000	4,5	66,0	1	1
9	CuSO ₄	27220	0	56,0	2	1
9	CuSO ₄	27220	0	56,0	2	1
10	CuSO ₄	32246	0	56,0	2	3
11	CuSO ₄	0	8625	0,4	0	0

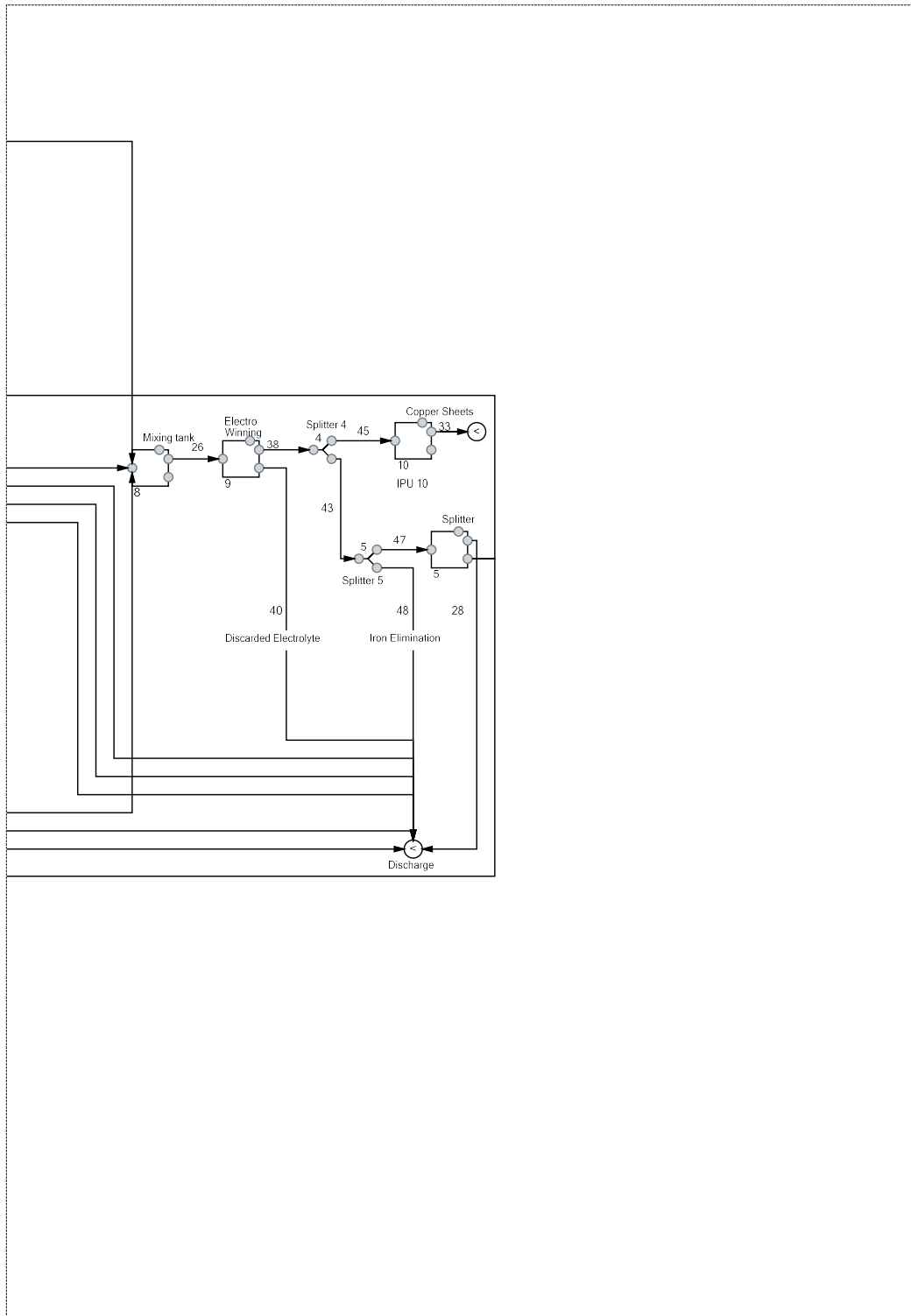
Table 6.2: Information about WW streams from various processes used for modelling

Ithaca Stream No.	Compound	Batch L	Overflow $L h^{-1}$	Concentration $g L^{-1}$	Services No. per year	Machines No.
1	$CuC_4H_4O_6$	2300	30	2,8	66	1
1	$CuC_4H_4O_6$	2300	30	2,8	66	1
1	$CuC_4H_4O_6$	2300	30	2,8	66	1
12	$CuC_4H_4O_6$	2500	56	2,8	52	3
12	$CuC_4H_4O_6$	2500	56	2,8	52	3
12	$CuC_4H_4O_6$	2500	56	2,8	52	2
12	$CuC_4H_4O_6$	2500	56	2,8	52	2
15	$CuSO_4$	600	0	14,0	52	3
14	$CuSO_4$	540	20	16,0	66	1
14	$CuSO_4$	540	20	16,0	66	1
14	$CuSO_4$	540	20	16,0	66	1
18	$CuSO_4$	1060	0	3,0	36	1
17	$CuSO_4$	1000	30	18,0	36	3
16	$CuSO_4$	950	30	18,0	36	3
13	$CuSO_4$	500	0	3,0	36	1
18	$CuSO_4$	1060	0	3,0	36	1
17	$CuSO_4$	1000	30	18,0	36	2
16	$CuSO_4$	950	30	18,0	36	2
13	$CuSO_4$	500	0	3,0	36	1
2	$CuSO_4$	320	34	18,5	2	1
5	$CuSO_4$	550	34	18,5	1	3
5	$CuSO_4$	550	34	18,5	1	3
5	$CuSO_4$	550	34	18,5	1	4
5	$CuSO_4$	550	34	18,5	1	4
4	$CuSO_4$	830	14,5	28,0	12	3
4	$CuSO_4$	830	14,5	28,0	12	3
4	$CuSO_4$	830	14,5	28,0	12	2
4	$CuSO_4$	830	14,5	28,0	12	2
3	$CuCl_2$	3000	80	129,6	-	2
3	HCl	-	-	138,5	-	-
29	H_2O	-	208,3	0,0	-	-



- page 1 -

Figure 6.1: Model in ITHACA - page 1



- page 2 -

Figure 6.2: Model in ITHACA - page 2

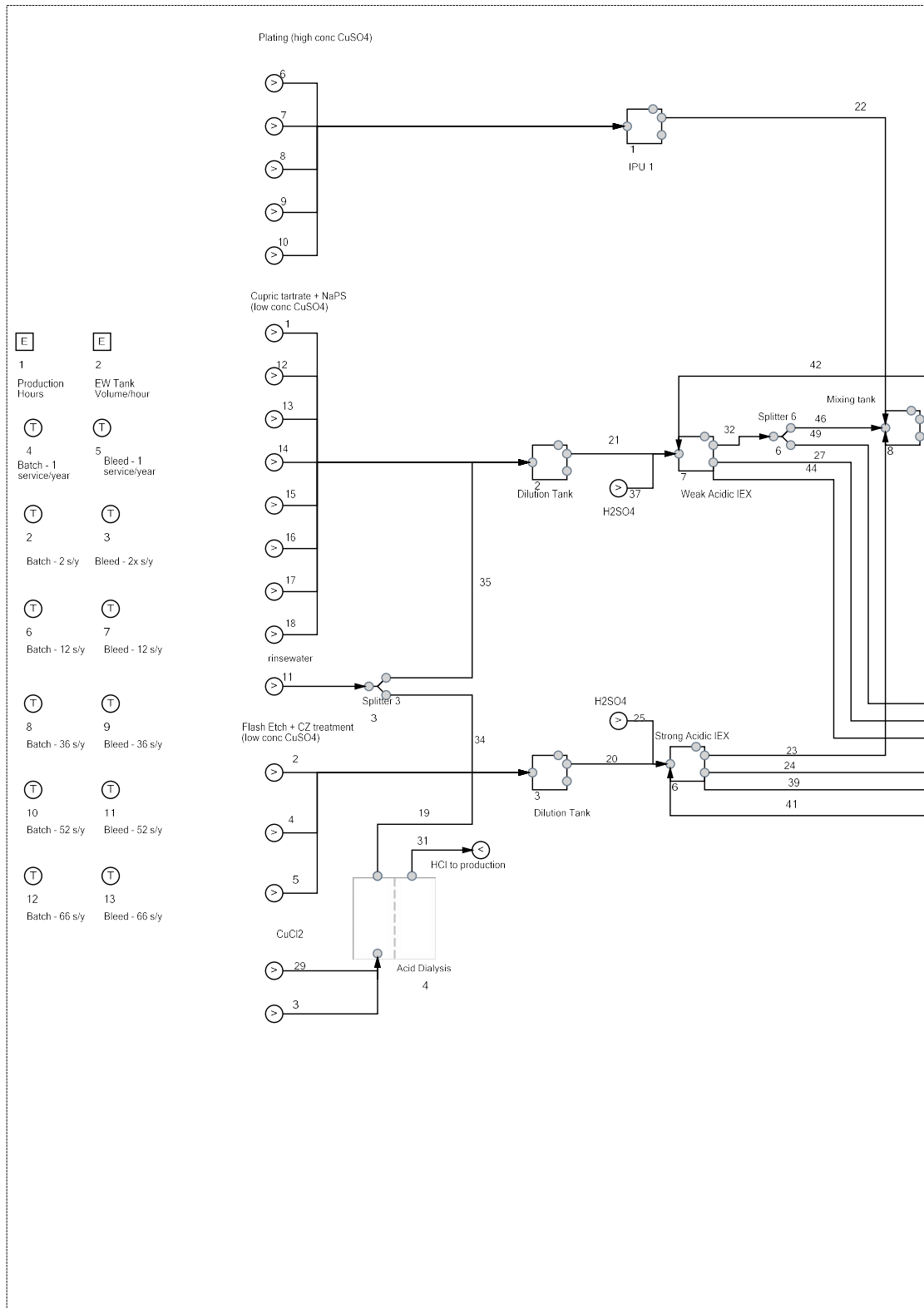


Figure 6.3: Simulation framework in ITHACA - page 1

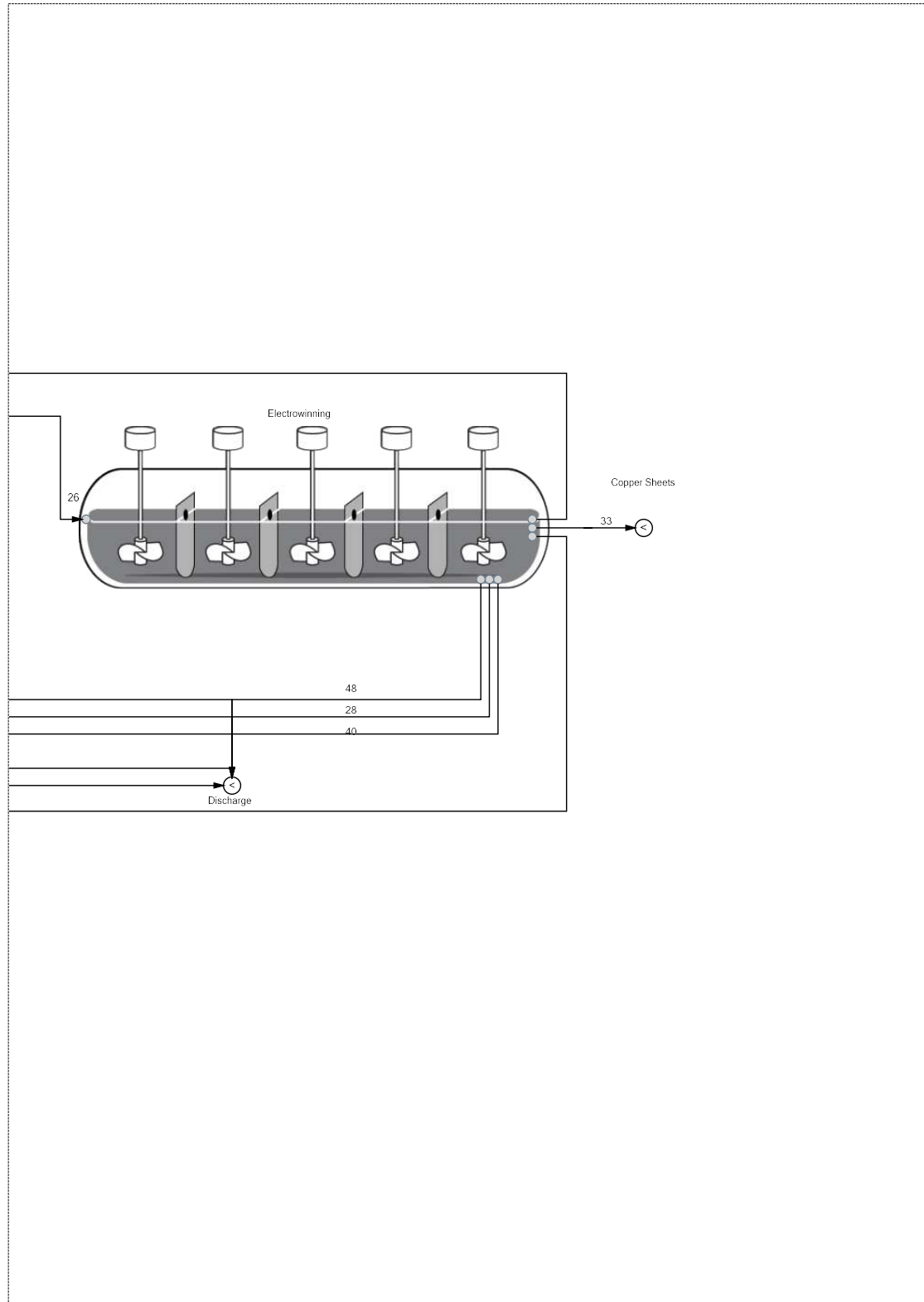


Figure 6.4: Simulation framework in ITHACA - page 2