

Master's Thesis in Chemical Engineering
Chalmers University of Technology

**Dynamic Simulation of Lignin
Composition Transients During
Wood Species Switching at
Södra Cell Mönsterås**

Francis Gillet

Department of Chemistry and Chemical Engineering
Chalmers University of Technology
Gothenburg, Sweden, 2026

Industrial Supervisors: Johanna Olsson (Lignin Specialist, Södra)
Anders Åkesjö (Simulation Specialist, Södra)

Academic Examiner: Prof. Derek Creaser
Chemical Engineering, Chalmers

Host Company: Södra Cell Mönsterås (SCMS)

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Abstract

Södra Cell Mönsterås (SCMS) is a kraft pulp mill located in Mönsterås, Sweden, operated by the forest-owner cooperative Södra. In the kraft process, wood chips are chemically cooked under high temperature and pressure in an alkaline solution, dissolving the lignin and liberating cellulose fibres as pulp. The dissolved organic material forms black liquor, which is concentrated and burned in the recovery boiler to regenerate the cooking chemicals and produce steam. SCMS is unique in its ability to process both HW (Hardwood, primarily birch) and SW (Softwood, primarily pine and spruce) feedstocks, and is commissioning a large-scale lignin separation facility — among the largest of its kind globally — to produce separated kraft lignin as a bio-based material for industrial applications.

Lignin, a structural biopolymer found in wood cell walls, has traditionally been burned for energy recovery during chemical regeneration. Growing demand for bio-based materials has created a market for separated kraft lignin. However, hardwood and softwood lignins differ significantly in molecular structure and downstream application potential and must be kept separate to maintain reliable product quality. When the mill switches between wood species, a prolonged transient period occurs during which mixed-species black liquor propagates through the cooking, washing, and evaporation stages before reaching the lignin separation unit, producing lignin of uncertain specification during the transition period.

This thesis develops a dynamic process simulation model using the **ExtendSim** platform and the in-house **PulpMaster** block library to predict and quantify the lignin composition transient during wood species transitions. Xylan — a hemicellulose present at markedly different concentrations in hardwood (≈ 12.5 g/kg) and softwood (≈ 2.8 g/kg) weak black liquor — is used as a compositional tracer to indicate whether the liquor at any given point in the process is hardwood-derived, softwood-derived, or a mixture of the two. A 7-effect falling-film evaporation section was constructed and connected to the existing mill model, and the model was validated against 34 laboratory xylan measurements collected during a real HW \rightarrow SW \rightarrow HW transition.

The best-matching scenario (LM tank bypass with 75% recirculation) achieved come-up and come-down root-mean-square errors of 1.00 g/kg and 0.88 g/kg respectively, evaluated separately over the rising transient (0–100 h, 17 measurement points) and the falling transient (186–250 h, 13 measurement points), both within ≈ 9 –10% of the full HW-to-SW xylan concentration range of 9.7 g/kg. These results confirm the model

as an accurate predictor of the composition transient. A key process discovery during validation was that the plant was operating with an intermediate liquor tank bypassed for maintenance, which reduced the come-up transition time T_{95} by 15 hours. Four operating scenarios were evaluated and compared against the observed baseline; the results show that targeted operational adjustments — in particular reducing tank fill levels before a transition and managing the recirculation rate — can substantially shorten the mixed-species transient and increase the volume of on-specification prima lignin product per transition.

Keywords: kraft pulping, lignin, dynamic simulation, wood species transition, hardwood, softwood, xylan, ExtendSim, PulpMaster, black liquor, evaporation, residence time, lignin separation, Södra Cell.

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Nomenclature and Abbreviations

Mill and Process Locations

- SCMS** Södra Cell Mönsterås — the kraft pulp mill in Mönsterås, Sweden, operated by Södra.
- RTDB** Real-Time Database — the ABB-developed process historian at SCMS, providing sub-minute logged measurements of tank levels, flows, temperatures, and dry solids.

Wood Species

- HW** Hardwood — at SCMS, primarily birch (*Betula* spp.).
- SW** Softwood — at SCMS, primarily Norway spruce (*Picea abies*) and Scots pine (*Pinus sylvestris*).

Process Liquor Streams

The black liquor progressively increases in dry solids content as it moves through the evaporation plant. The following abbreviations denote the liquor at different concentration stages.

WBL	Weak Black Liquor (<i>Tunnlut</i>) — spent cooking liquor leaving the brown stock washing plant at approximately 15% dry solids (DS). This is the feed to the evaporation plant. Also denoted LT in the tank farm (see below).
LT	Tunnlut from the digester (<i>Tunnlut från Kokeri</i>) — equivalent to WBL; denotes the weak black liquor arriving directly from the cooking section before entering the evaporation tank farm.
LB	Mixed Liquor (<i>Blandlut</i>) — WBL mixed with intermediate liquor (LM/LTJM), producing a blended stream.
LM	Intermediate Liquor (<i>Mellanlut</i>) — black liquor at an intermediate concentration stage in the evaporation train. The LM1 tank is the primary intermediate storage vessel and the dominant holdup volume identified in this thesis.
LTJM	Intermediate-Thick Liquor (<i>Mellantjocklut</i>) — black liquor at a higher concentration stage than LM, in the range 44–52% DS. LTJM4 denotes the associated recirculation tank.
SBL	Strong Black Liquor (<i>Tjocklut</i>) — concentrated black liquor leaving the evaporation plant at approximately 70–72% DS.
BL	Black Liquor — general term for the dissolved organic and inorganic material extracted from the digester and washing stages, at any concentration.

Process Equipment and Concepts

BT	Blow Tank (<i>Blåstank</i>) — buffer vessel between the digester and the washing stages, where the pulp pressure is released to atmospheric conditions.
CSTR	Continuously Stirred Tank Reactor — an idealised perfectly mixed vessel. All tank volumes in the simulation model are approximated as CSTRs.
DS	Dry Solids — mass fraction of dissolved and suspended solids in a liquor stream, expressed as a percentage (%DS). The complement ($100 - \%DS$) gives the water content. A WBL feed entering the evaporation plant is typically 15% DS; the SBL leaving is 70–72% DS.
MPC	Model Predictive Control — an advanced process control strategy that uses a process model to optimise control actions over a future time horizon.

Statistical Metrics

RMSE	Root Mean Square Error — measure of the average magnitude of simulation error relative to laboratory measurements.
MAE	Mean Absolute Error — measure of the average absolute deviation between simulated and measured values.
T₉₅	The time elapsed from a species switch until the xylan concentration at the lignin separation feed reaches 95% of its new steady-state value.
T₈₀	Same as T ₉₅ but for 80% completion, used where the simulation window does not extend to full 95% completion.

Chemical Abbreviations

G	Guaiacyl — monolignol unit derived from coniferyl alcohol, carrying one methoxy group. The dominant unit in softwood lignin.
S	Syringyl — monolignol unit derived from sinapyl alcohol, carrying two methoxy groups. Present alongside G units in hardwood lignin.
H	p-Hydroxyphenyl — monolignol unit derived from p-coumaryl alcohol, carrying no methoxy groups. Present in trace amounts.
GX	Glucuronoxylan — the dominant hemicellulose in hardwood, constituting 20–30% of dry wood mass.
AGX	Arabinoglucuronoxylan — the xylan form found in softwood, present at only 5–10% of dry wood mass.
LCC	Lignin–Carbohydrate Complex — covalent linkages between lignin and hemicellulose within the wood cell wall.
MeGlcA	4-O-methyl-glucuronic acid — a substituent on the xylan backbone at approximately every 10th xylose unit.

1 Introduction

1.1 Background

The kraft process is a chemical pulping method in which wood chips are cooked under high temperature and pressure in an alkaline solution of sodium hydroxide and sodium sulphide, breaking down the lignin matrix that binds the wood fibres and liberating the cellulose fibres as pulp. The cooking liquor, which dissolves the lignin together with hemicelluloses and other wood extractives, becomes a dark liquid known as black liquor. This black liquor is subsequently concentrated in the evaporation plant and combusted in the recovery boiler to regenerate the cooking chemicals and produce process steam.

Södra Cell Mönsterås (SCMS) is a kraft pulp mill located in Mönsterås, Sweden, operated by the forest-owner cooperative Södra. The mill is unique in its ability to process both hardwood (HW, primarily birch, *Betula* spp.) and softwood (SW, primarily Norway spruce, *Picea abies*, and Scots pine, *Pinus sylvestris*) feedstocks, switching between species based on market conditions and wood availability. Kraft pulp is the mill's primary product; alongside pulp production, SCMS is commissioning a large-scale lignin separation facility — among the largest of its kind globally — to produce separated kraft lignin as a bio-based material for industrial applications [1, 2].

In the global transition toward a more sustainable, bio-based economy, lignin is increasingly recognised as a valuable renewable resource. As the second most abundant natural polymer on Earth, kraft lignin represents a significant opportunity for producing bio-based materials, chemicals, and fuels. However, lignin derived from softwood and hardwood differs significantly in its molecular structure and application potential. Softwood lignin is composed primarily of guaiacyl (G) units, whereas hardwood lignin contains a mixture of guaiacyl (G) and syringyl (S) units, with trace amounts of p-hydroxyphenyl (H) units [3]. This structural difference directly affects the downstream application potential of the separated lignin product, and the two lignin types must be kept separate to maintain reliable product quality and specification.

When the mill transitions from cooking one wood species to another, the black liquor composition does not change instantaneously downstream from the pulp digester. The large volumes of process liquor circulating through the digester, brown stock washing, and evaporation stages create a prolonged transient period during which the lignin in the black liquor is a mixture of both hardwood and softwood. Understanding, predict-

ing, and ultimately minimising this mixed-species transient can improve operation and product quality.

1.2 Problem Statement and Objectives

The central research questions of this thesis are:

- *How does the lignin composition in the black liquor at the lignin separation feed point evolve over time during a wood species transition at Södra Cell Mönsterås?*
- *How can dynamic process simulation be used to predict and minimise the duration of the mixed-species transient period?*

To address these questions, the following objectives were pursued:

1. Conduct a literature review of kraft pulping chemistry, hardwood versus softwood lignin structure, and dynamic process simulation methodologies for pulp mills.
2. Develop a thorough understanding of the SCMS process flow from wood chip feeding through cooking, washing, and evaporation to the lignin separation feed point.
3. Update and extend the existing SCMS ExtendSim simulation model to track HW and SW lignin fractions (using xylan as a proxy) through all relevant process stages, including a newly built evaporation section.
4. Develop a calibration methodology for the simulation model, including a systematic approach to setting unknown process parameters using available RTDB data, operator knowledge, and iterative comparison against the observed transient behaviour.
5. Verify the simulation model against laboratory xylan concentration data measured during real wood species transitions at SCMS.
6. Use the verified model to evaluate and rank operational strategies for minimising the mixed-species transition period.

1.3 Industrial Relevance

This work directly supports Södra's commercial strategy for high-quality lignin production. During a wood species transition, lignin of uncertain or mixed specification is produced, which is difficult to sell reliably to customers with defined product requirements. By quantifying and minimising this transition time, the mill can:

- Reduce the volume of off-specification lignin produced during wood species changeovers.

- Improve planning of production schedules for the lignin separation plant and downstream customers.
- Gain a digital process model that can be used for operator training, scenario analysis, and future process control development.
- Lay the groundwork for model predictive control (MPC) integration targeting lignin product consistency.

1.4 Scope and Limitations

The simulation scope spans from the wood chip feed through the digester to the evaporation stage that feeds the lignin separation plant. The model is a lumped-parameter dynamic simulation and does not resolve spatial concentration gradients within individual process units. All tanks are assumed to be perfectly mixed (CSTR assumption); the motivation for this and its limitations are discussed in Section 5.5.

2 Theory

2.1 Kraft Pulping Chemistry

2.1.1 Process Liquor Compositions

The fresh cooking liquor in the kraft process is called white liquor, which is an aqueous solution of sodium hydroxide (NaOH) and sodium sulfide (Na₂S) produced in the chemical recovery cycle.

During woodchip cooking, under elevated temperature (180 °C) and pressure (11 bar(g)), white liquor diffuses into the woodchips and into the tracheid cell wall where the lignin is broken down and dissolved into the white liquor giving it a reddish black color. Cellulose fibers are released from the cell wall matrix and liberated as a suspension in the liquor. This spent white liquor is then called black liquor and is rich in tree oils, dissolved lignin, and a consortia of carbohydrates.

2.2 Lignin in the Tracheid Cell

Gymnosperms evolved from bryophyte ancestors approximately 350 million years ago, developing vascular tissue to grow upright and compete for sunlight. Lignin biosynthesis in the tracheid cells is believed to proceed through a stochastic radical-coupling mechanism, producing the highly heterogeneous polymer network observed in mature wood cell walls [4].

Hemicelluloses act as a connective tissue between the lignin matrix and the cellulose fibrils. Figure 2.1 shows the molecular architecture of the wood cell wall at the microfibril scale: crystalline cellulose chains (blue) form the load-bearing scaffold, coated by glucomannan (green) and xylan (pink), with lignin (grey) filling the surrounding matrix and covalently linking to the hemicelluloses via lignin-carbohydrate complexes (LCC).

2.3 Xylan Chemistry

2.3.1 Structure of Xylan in Hardwood and Softwood

Xylans are the dominant hemicelluloses in hardwood (22–28% of dry wood mass) and the second most abundant hemicellulose in softwood (8–9% of dry wood mass) [6]. The

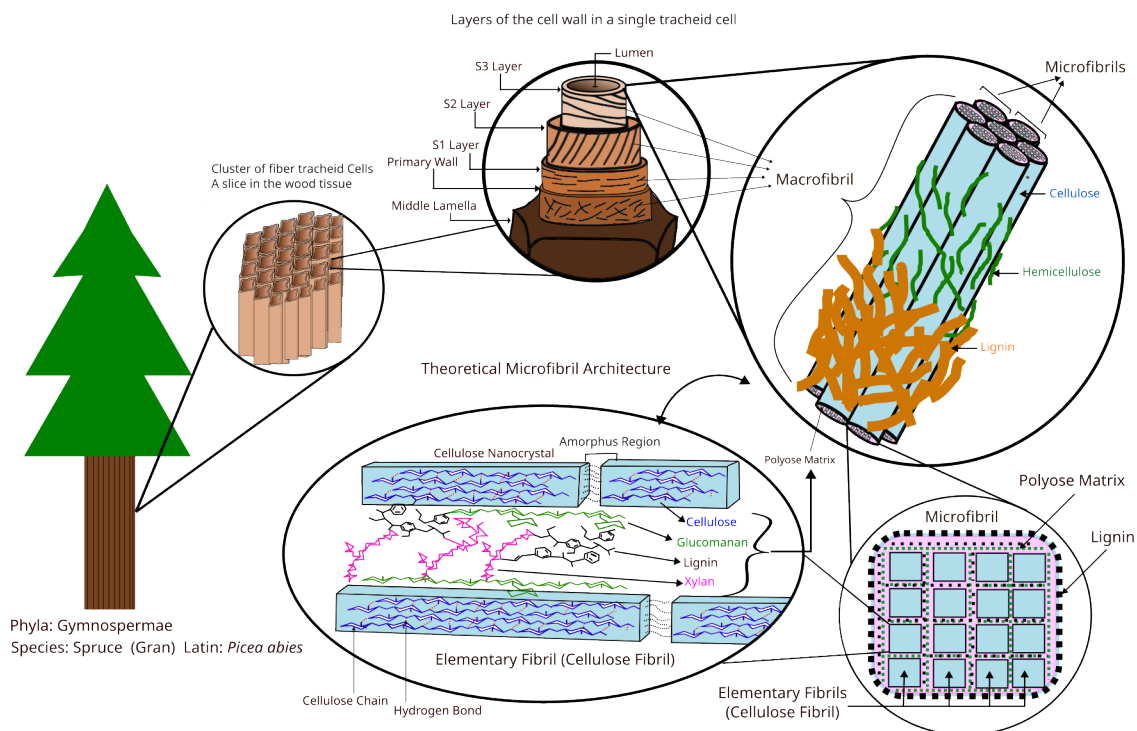


Figure 2.1: Hierarchical structure of the softwood tracheid cell (*Picea abies*). From left: tree → cluster of fibre tracheid cells in wood tissue → cell wall layers (Middle Lamella, S1, S2, S3) → microfibril showing cellulose, hemicellulose and lignin → theoretical microfibril architecture with crystalline cellulose core, glucomannan, xylan and amorphous lignin matrix.

repeat unit structures of both types are shown in fig. 2.3; the key structural differences between species are:

Hardwood glucuronoxylan (GX): A linear backbone of β -1,4-linked D-xylopyranose units, with α -D-4-O-methyl-glucuronic acid (MeGlcA) substituents at approximately every 10th xylose unit (degree of substitution ≈ 0.1). In hardwood, acetyl groups at C2 and/or C3 are also present, accounting for the acetic acid liberated during kraft cooking. Glucuronoxylan constitutes 20–30% of dry HW mass.

Softwood arabinoglucuronoxylan (AGX): The same β -1,4-xylan backbone, but with both MeGlcA (at C2, lower frequency) and α -L-arabinofuranose (at C3) substituents. Acetyl groups are absent in softwood xylan. AGX constitutes only 5–10% of dry SW mass.

The large quantitative difference in xylan content between HW and SW is illustrated in table 2.1, which gives the bulk chemical composition of representative commercial species. In hardwood, essentially all of the xylan fraction is glucuronoxylan (GX), accounting for 22–28% of dry wood mass. In softwood, the xylan fraction consists almost

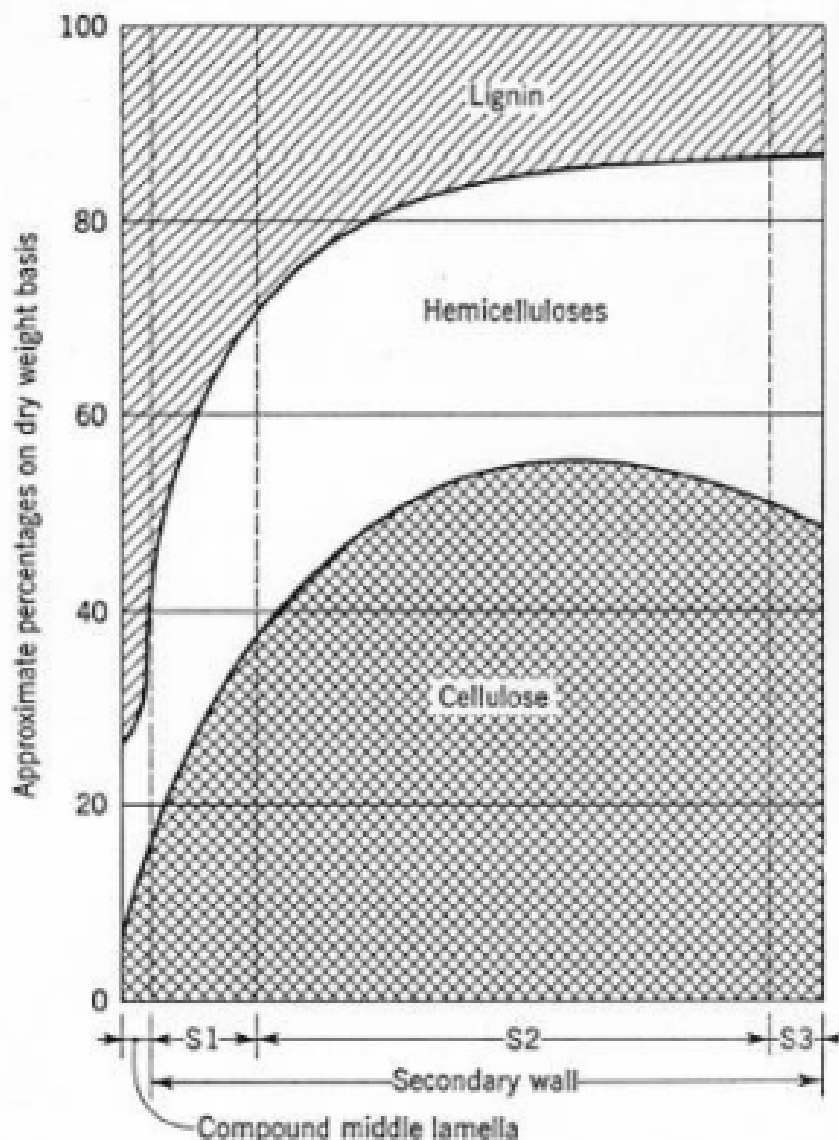


Figure 2.2: Distribution of cellulose, hemicelluloses and lignin across the fibre cell wall. Originally from Panshin and de Zeeuw (1980), as reproduced in [5].

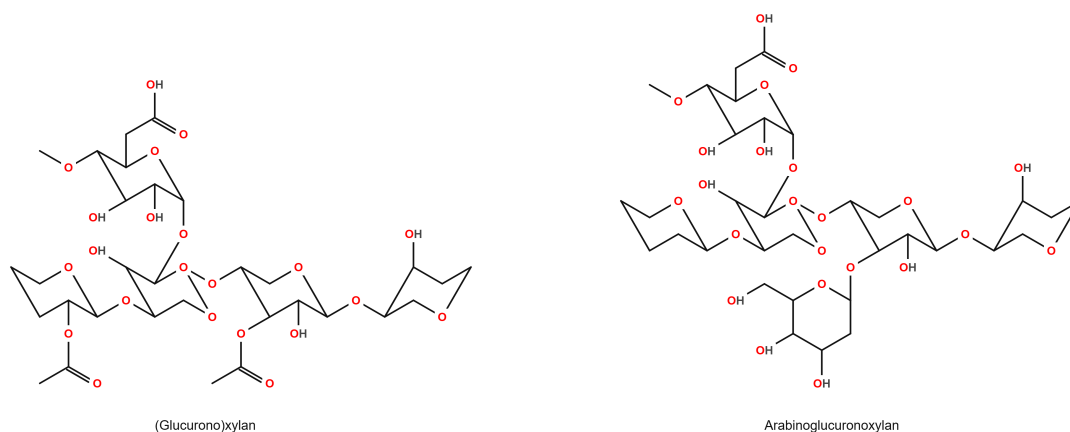
entirely of arabinoglucuronoxylan (AGX), at only 8–9% of dry wood mass; there are no other significant xylan types present in these commercial species. GX and AGX are therefore not sub-fractions of the xylan pool; each constitutes the whole xylan fraction in its respective wood type. Glucomannan shows the inverse pattern, dominating the hemicellulose fraction in softwood (~16%) but nearly absent in hardwood (<4%). This contrast is the chemical foundation for using xylan and glucomannan as species tracers in the black liquor (see section 2.3.4).

2.3.2 Xylan Dissolution During Kraft Cooking

Xylan dissolves into the cooking liquor by two simultaneous mechanisms:

Table 2.1: Chemical composition of selected wood species (% of dry wood mass). Data from [4].

Species	Extractives	Lignin	Cellulose	Glucomannan	Xylan	Other poly-sacch.	Other
<i>Softwoods</i>							
Norway spruce (<i>Picea abies</i>)	1.7	27.4	41.7	16.3	8.6	3.4	0.9
Scots pine (<i>Pinus sylvestris</i>)	3.5	27.7	40.0	16.0	8.9	3.6	0.3
<i>Hardwoods</i>							
Birch (<i>Betula verrucosa</i>)	3.2	22.0	41.0	2.3	27.5	2.6	1.4
Beech (<i>Fagus sylvatica</i>)	1.2	24.8	39.4	1.3	27.8	4.2	1.3
River red gum (<i>Eucalyptus camaldulensis</i>)	2.8	31.3	45.0	3.1	14.1	2.0	1.7
Red maple (<i>Acer rubrum</i>)	3.2	25.4	42.0	3.1	22.1	3.7	0.5



(a) Hardwood glucuronoxylan (GX). The β -1,4-xylose backbone carries MeGlcA substituents and acetyl groups at C2/C3.

(b) Softwood arabinoglucuronoxylan (AGX). The same xylose backbone carries MeGlcA and arabinofuranose substituents; acetyl groups are absent.

Figure 2.3: Repeat unit structures of (a) hardwood glucuronoxylan and (b) softwood arabinoglucuronoxylan. The absence of acetyl groups and presence of arabinose in AGX reduces its solubility contrast with cellulose, making it a less effective process tracer than GX.

Alkaline Peeling

Peeling is a β -elimination reaction that proceeds from the reducing end of a polysaccharide chain. Under alkaline conditions, the reducing terminal unit is converted to an enediol, which undergoes β -elimination to release a sugar acid (isosaccharinic acid) and regenerate a new reducing end. The cycle then repeats on the exposed next unit.

Each peeling step shortens the chain by one sugar residue. For xylan, peeling releases xylose units as xyloisosaccharinic acid into the cooking liquor [7]. The rate of peeling increases with temperature (activation energy ≈ 100 – 130 kJ mol^{-1}) and with OH^- concentration.

Importantly, peeling is considerably less effective for xylan than for cellulose. The substituents on the xylan backbone MeGlcA at C2 and acetyl groups at C2/C3 interfere

with the β -elimination mechanism, making xylan more resistant to alkaline degradation than cellulose [4]. This relative stability means that a significant fraction of xylan survives the cook and is dissolved intact into the black liquor, which is what makes it a useful compositional tracer. The acetyl groups are themselves cleaved under alkaline conditions, releasing acetic acid into the cooking liquor as a by-product.

Stopping Reaction

Competing with peeling is the **stopping reaction**: the enediol intermediate at the reducing end undergoes intramolecular rearrangement to form a stable metasaccharinic acid end group that cannot undergo further β -elimination. This terminates the peeling sequence at that chain end. The stopping reaction also increases with temperature, but with a lower activation energy than peeling, so at very high temperatures the rate of the stopping reaction exceeds that of peeling, resulting in a lower total yield loss.

Alkaline Hydrolysis

Direct OH^- -mediated hydrolysis of glycosidic bonds cleaves the xylan backbone at internal positions, creating new chain ends that then become new sites for peeling. Hydrolysis is slow at cooking temperatures but becomes significant at extended cook times or during the residual phase.

2.3.3 Xylan Reprecipitation

A distinctive feature of hardwood xylan is its ability to reprecipitate onto the cellulose fiber surface during the later stages of kraft cooking [8]. As the temperature increases and ionic strength rises, dissolved xylan oligomers become less soluble and adsorb onto the hydrogen-bond-rich cellulose surface. This reprecipitation:

- **Increases pulp yield** beyond what simple dissolution kinetics would predict.
- **Improves fiber bonding** in the final pulp (xylan acts as a bonding agent between fibres), increasing strength properties of HW kraft pulp.
- **Reduces xylan concentration in black liquor** relative to the amount dissolved during cooking, since a fraction is retained on the fiber.

Softwood xylan (AGX) is less prone to reprecipitation, partly because the arabinose substituents disrupt the ordered conformation needed for cellulose surface adsorption. This difference contributes to the higher dissolved xylan concentration in HW black liquor compared to SW black liquor at comparable cooking conditions, making xylan an effective compositional marker (see section 2.3.4).

It is important to note that although reprecipitation does reduce the dissolved xylan concentration in HW black liquor relative to the total amount solubilised during cooking, it does not reverse the fundamental species contrast. Hardwood contains 22–28% xylan on a dry-wood basis compared to only 8–9% in softwood (table 2.1), so even after accounting for reprecipitation losses, the dissolved xylan concentration in HW black liquor remains substantially higher than in SW black liquor. The fraction retained on the pulp fibre is a relatively small portion of the large initial HW xylan pool, and the remaining dissolved xylan signal in the black liquor is still readily detectable and reliable as a species tracer.

2.3.4 Xylan as a Compositional Tracer in Black Liquor

The combination of (i) high glucuronoxyxylan content in HW ($\sim 20\text{--}30\%$), (ii) low AGX content in SW ($\sim 5\text{--}10\%$), and (iii) limited xylan reprecipitation in HW compared to cellulose retention, means that the xylan concentration in weak black liquor differs substantially between HW and SW steady-state operation. This large and reproducible contrast makes xylan concentration an ideal process tracer for detecting the mixing front during a wood species transition.

Xylan is stable in black liquor (BL) under evaporation conditions (temperatures $< 150^\circ\text{C}$); although BL remains alkaline at pH 11–12, the significantly lower temperature compared to digester conditions is sufficient to arrest further peeling. This stability means that the xylan concentration at any point downstream of the washing plant is directly reflective of the upstream cooking conditions at the time the liquor entered the system.

2.3.5 Xylan Concentration During Wood Species Transitions

During a HW \rightarrow SW transition, the xylan concentration in the weak black liquor (WBL) — the dilute black liquor leaving the washing plant — decreases from its HW steady-state level toward the (lower) SW steady-state level. The rate of this change at any given measurement point is governed by the residence time distribution of the process vessels upstream of that point exactly what the dynamic simulation model is designed to capture (see chapter 4).

2.4 Lignin Structure and Material Properties

2.4.1 Monolignol Building Blocks and Inter-Unit Linkages

Lignin is an amorphous, three-dimensional aromatic polymer derived from radical coupling of three monolignols: p-coumaryl alcohol (gives H units), coniferyl alcohol (gives

G units), and sinapyl alcohol (gives S units) [1], shown in fig. 2.4. The coupling is enzyme-initiated but chemically random, producing a highly heterogeneous polymer with a distribution of inter-unit linkages.

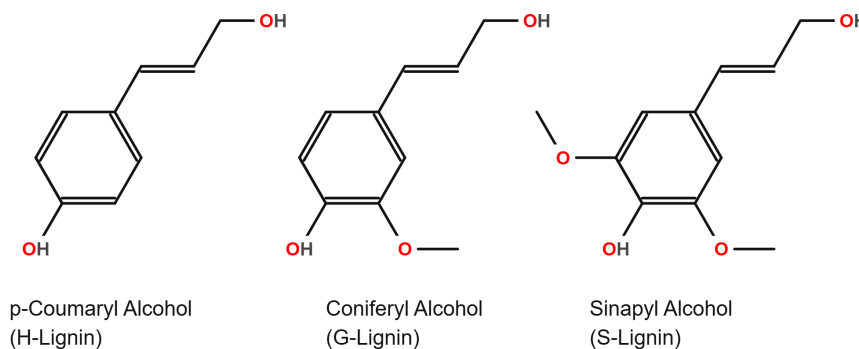


Figure 2.4: The three monolignol precursors of lignin. From left: p-coumaryl alcohol (H unit, no methoxy groups), coniferyl alcohol (G unit, one methoxy group), and sinapyl alcohol (S unit, two methoxy groups). Softwood lignin consists primarily of G units, while hardwood lignin contains a mixture of G and S units.

2.4.2 Hardwood versus Softwood Lignin Composition

Softwood lignin is composed almost entirely of G units ($S/G \approx 0$), whereas hardwood lignin contains a mixture of G and S units ($S/G = 1-3$ depending on species) with trace H units [3]. This structural difference affects delignification reactivity and downstream product properties [9], and is the chemical basis for why HW and SW lignins must be kept separate at the lignin separation plant.

2.4.3 Kraft Lignin Separation

The lignin separation process operates on the principle that lignin is ionised and dissolved in black liquor under alkaline conditions (pH 11–12). Separation is achieved by acidifying the black liquor with CO_2 , which lowers the pH and precipitates the lignin as a slurry. The slurry is then dewatered by pressure filtration and washed with dilute acid to recover sodium and sulphur, yielding an acid-washed lignin cake. The cake is subsequently dried to produce a yellowish-brown powder that can be further processed into pellets or used directly as a solid biofuel or chemical feedstock [10, 11].

2.5 Dynamic Process Simulation in Pulp Mills

2.5.1 Overview of Simulation Approaches

Dynamic process simulation differs from steady-state simulation in that it captures the time-dependent behaviour of process variables in response to disturbances or deliberate changes in operating conditions [12, 13]. Dynamic modelling of kraft digesters has been explored in the literature [14], and process simulation has been applied to lignin extraction from softwood pulping plants [15]; however no published model tracks HW/SW composition through the full evaporation and lignin separation chain as developed here. For this thesis, a dynamic model is essential because the wood species transition is inherently a transient phenomenon: the composition at any point in the mill changes continuously over many hours as the “old liquor” is displaced by the “new” liquor from the digester. Each storage tank and process vessel acts as a mixing volume that delays and smears the composition front; for a well-agitated tank of volume V with volumetric flow rate q , the mean hydraulic residence time is $\bar{t} = V/q$, which sets the characteristic time scale of the composition change at that point.

2.6 Summary and Literature Gaps

The literature review reveals the following gaps that this thesis addresses:

- No published dynamic model tracks HW/SW lignin composition through the full process chain from digester to lignin separation feed in an industrial kraft pulp mill.

3 Process Description

3.1 Södra Cell Mönsterås Overview

Södra Cell Mönsterås (SCMS) is a kraft pulp mill located in Mönsterås, Sweden, operated by the forest-owner cooperative Södra. The mill is unique in the industry in its ability to produce pulp from both hardwood (primarily birch, *Betula* spp.) and softwood (primarily spruce, *Picea abies*, and pine, *Pinus sylvestris*) depending on market conditions. Alongside pulp, SCMS is commissioning a large-scale lignin separation facility, among the largest of its kind in the world.

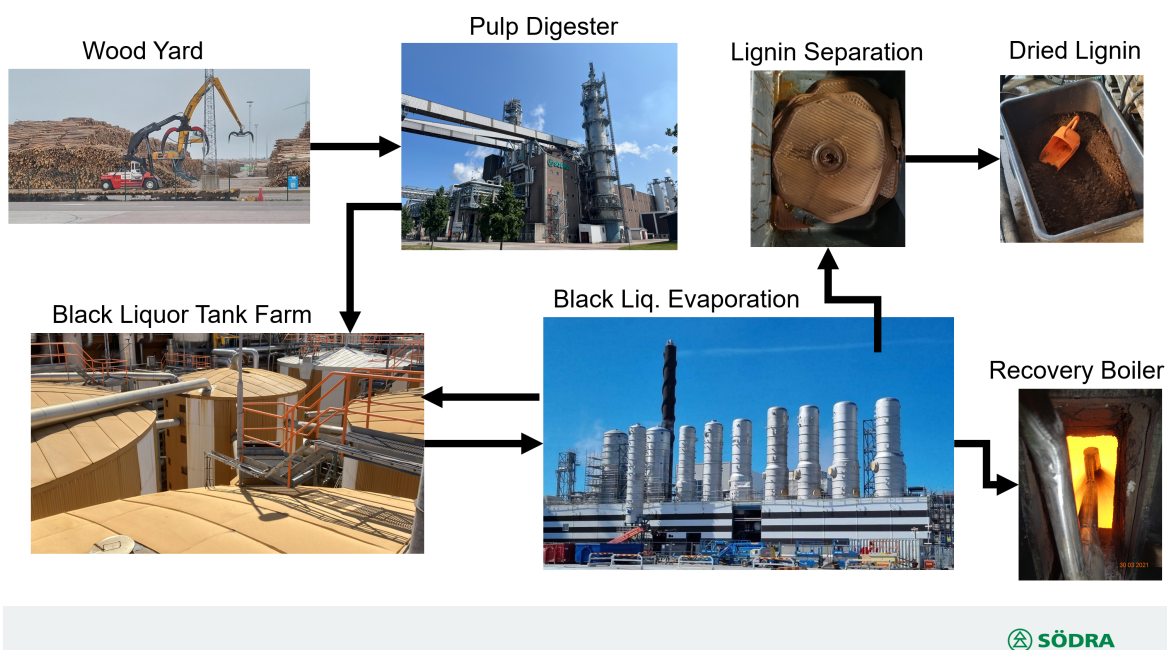


Figure 3.1: Overview of the lignin production process at Södra Cell Mönsterås. Wood chips enter at the wood yard and are cooked in the pulp digester; black liquor is collected in the tank farm and concentrated in the evaporation plant before a side-stream is fed to lignin separation, yielding dried lignin product. The remaining concentrated black liquor proceeds to the recovery boiler.

3.2 Cooking Stage (Digestern)

The digester is a 60 m tall pressurised vessel in which wood chips are chemically delignified at approximately 170 °C and 10 bar gauge pressure. White liquor (containing NaOH and Na₂S) is mixed with wood chips under these conditions; the cooking liquor diffuses into the tracheid cell walls, fragmenting and dissolving the lignin from the

cellulose-rich fibrils and liberating the cellulose fibres. Hemicelluloses in the cell walls also break down during cooking. The dissolved lignin, together with hemicelluloses, extractives, and degraded organic material, forms the weak black liquor (WBL) [16, 17].

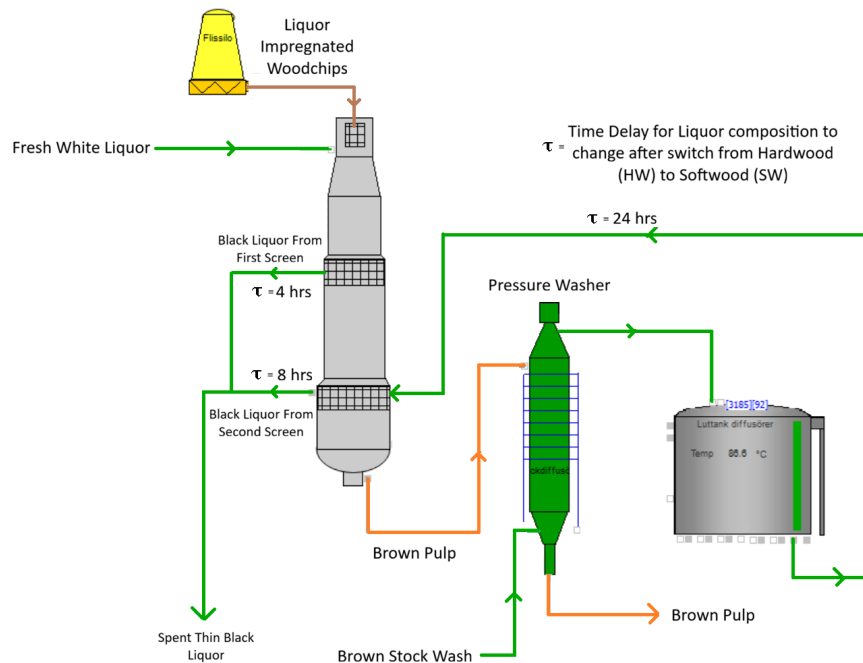


Figure 3.2: Block schema of the cooking section at SCMS. The continuous digester feeds liquor-impregnated wood chips at the top; black liquor is extracted at a first screen ($\tau = 4$ h after a species switch) and a second screen ($\tau = 6$ hours). Pulp discharges to a pressure washer and diffuser tank; the overall brown stock washing stage reaches the new species composition at $\tau = 24$ h.

3.2.1 Digester Transit Time During a Wood Species Transition

A key observation from mill data is the time required for a change in wood species at the chip feed to propagate through the digester and appear in the extracted black liquor. In a continuous digester, the chip column moves downward from the top feed through the impregnation and cooking zones to the discharge at the bottom; extraction screens at different heights allow liquor to be withdrawn at multiple points along this path.

During a softwood-to-hardwood (SW \rightarrow HW) transition, the following sequence was observed at SCMS:

1. Approximately **4 hours** after hardwood chips begin entering the digester, dissolved hardwood lignin starts to appear at the *first (upper) digester extraction screen*. Before this point the extracted black liquor still carries a softwood composition.

2. Approximately **8 hours** after the feed switch, hardwood lignin reaches the *lower (bottom) extraction screen*. This marks the point at which the advancing hardwood chip column has passed through the full active cooking zone.
3. During the intermediate period between approximately 4 h and 8 h after the switch, a roughly 50/50 blend of hardwood and softwood lignin is extracted from the digester and forwarded to the weak black liquor (tunnlut) storage tanks upstream of the evaporation plant.

These observations indicate that the digester acts as an approximately plug-flow vessel for the solid chip phase, with a transit time of roughly 4 h through the upper cooking zone and 8 h through the full cooking zone height. The 4-hour window of mixed-species extraction corresponds to the vertical height of chip column inside the digester that is simultaneously occupied by both old-species (SW) and new-species (HW) chips at the time of extraction.

This digester transit delay represents the *first contribution* to the overall wood species transition time and sets the earliest possible time at which composition changes can appear downstream in the evaporation and lignin separation sections.

3.3 Blow Tank (Blåstanken)

After cooking, the pulp slurry is discharged through a blow valve into the blow tank, where the conditions are released to atmospheric temperature and pressure. The blow tank acts as a buffer between the digester and the subsequent washing stages. SCMS is equipped with two blow tanks to separate hardwood fibers and softwood fibers based off fiber length.

3.4 Brown Stock Washing (Tvättstationen)

Brown stock washing separates the dissolved organic and inorganic material (black liquor) from the cellulose fibers using a counter-current washing scheme. The weak black liquor extracted from washing the pulp is collected in a series of tanks and sent to the evaporation plant along with the black liquor from the digester.

Mill observations from a SW→HW transition indicate that approximately **24 hours** after hardwood chips begin entering the digester, the brown stock washing plant has fully transitioned to a hardwood lignin composition in its extracted black liquor. This 24-hour figure encompasses the sum of the digester transit time (4 h to 8 h; see section 3.2.1), the pulp residence time in the blow tank, and the displacement of old-species filtrate through all washing stages. It therefore sets the earliest time at which the WBL

feed to the evaporation plant can be considered purely hardwood-derived under normal operating conditions.

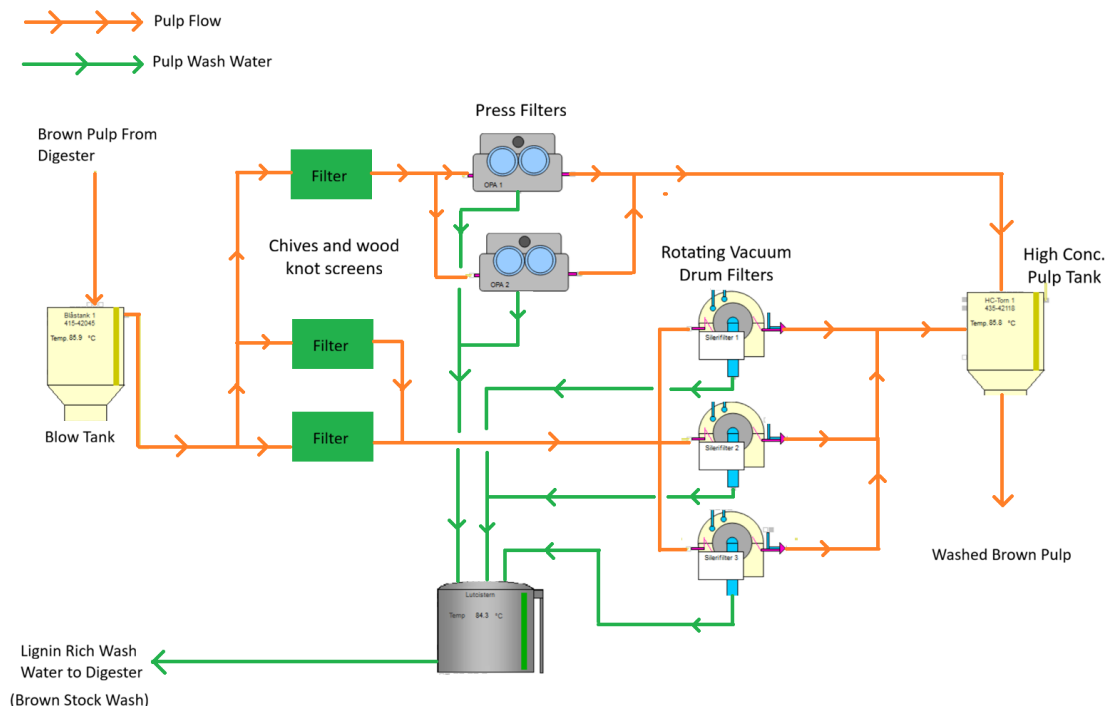


Figure 3.3: Block schema of the brown stock washing section (Sileri) at SCMS. Brown pulp from the digester enters via the blow tank (Blåstank, BT) and is washed in two parallel lines, each consisting of a drum filter (Filter) followed by a drum washer (DW). The partially washed pulp then passes through two oxygen pre-delignification washers (OPA 1, OPA 2) before three pressure diffuser filters (Silenfilter 1–3, SF) and a high-consistency tower (HC-Torn). Pulp wash water (green arrows) flows counter-currently against the pulp flow (orange arrows), maximising black liquor displacement efficiency. Lignin-rich wash filtrate is collected and returned to the digester via the liquor cistern (Lutcistern). Washed brown pulp exits at the right for further processing in the oxygen delignification and bleaching stages.

3.5 Evaporation Plant (Indunstningsanläggningen)

The evaporation plant concentrates the weak black liquor from approximately 15 % dry solids (DS) at the washing plant outlet to approximately 70 %–72 % DS. Where it is sent to a superconcentrator that concentrates the liquor to 80% DS this concentrated black liquor is sent to the recovery boiler for combustion and chemical regeneration. The evaporation is accomplished using multiple heat exchanger effects, where the black liquor evaporates as a falling-film evaporator train. where steam condenses on one side of heat exchanger surfaces and evaporates water from the liquor on the other side.

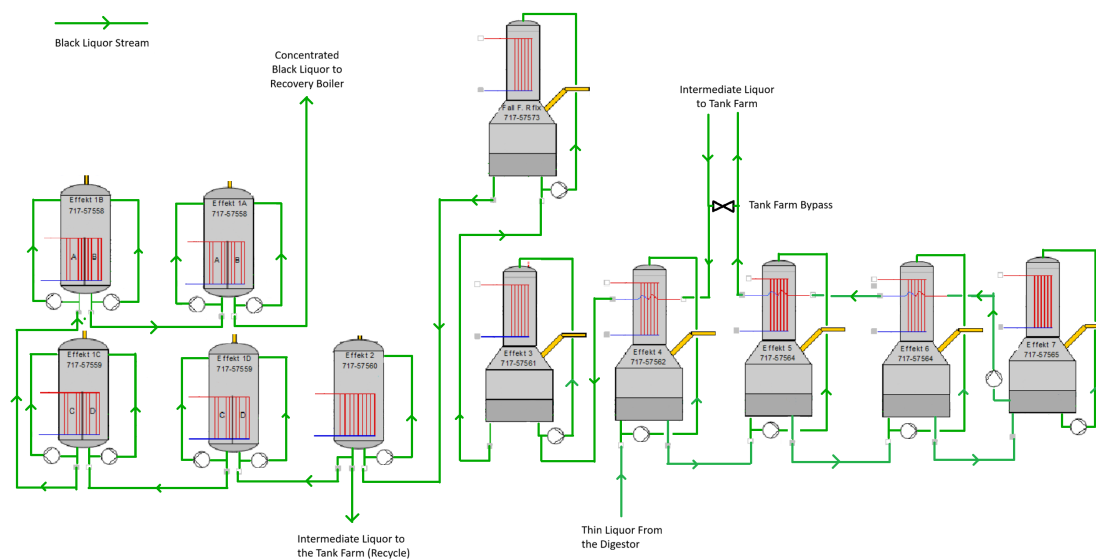


Figure 3.4: Block schema of the evaporation plant (Indunstningen) at SCMS. Thin black liquor enters from the digester on the right; the seven falling-film evaporator effects concentrate the liquor progressively as it moves left. Intermediate streams are diverted to the tank farm or to lignin separation feed, and concentrated black liquor exits to the recovery boiler.

3.5.1 Multi-Effect Evaporator Train

3.5.2 Weak Black Liquor (WBL) Storage Tank

Prior to entering the evaporator, the weak black liquor passes through a series of intermediate storage tanks that buffer flow from both the digester and the washing plant into the evaporation section. These tanks represent significant holdup volumes and are a major contributor to the overall species transition delay, as old-composition liquor must be displaced before the new-species composition reaches the evaporator feed.

3.5.3 Effect Sumps

In a falling-film evaporator, liquor is pumped to a distribution plate at the top of the steam tubes, from which it flows downward as a thin film. Steam condenses on the outside of the tubes, evaporating water from the falling liquor film. Each effect body holds a small volume of liquor in its sump; the volume of each sump was estimated from technical drawings of the individual effects. Although this holdup is minor compared to the storage tanks, it is included in the model and contributes a small additional delay to the composition transient.

4 Methodology

4.1 Overview of Approach

The methodology of this thesis consists of four interrelated components: (1) dynamic process simulation using ExtendSim and the PulpMaster library, (2) xylan-based model verification against laboratory data, (3) model calibration using plant operating data. (4) scenario analysis for transition optimization.

4.2 Simulation Platform: ExtendSim

4.2.1 ExtendSim Software

ExtendSim is a block-diagram based continuous and discrete-event simulation platform. The SCMS simulation model uses the continuous simulation mode, where differential equations are integrated using a fixed time-step Euler method. The PulpMaster library is an in-house collection of ExtendSim block types developed at Södra Cell, designed to represent all major unit operations in a kraft pulp mill. Each block communicates via a standardized flow vector with a fixed number of components defined by the global parameter `GlobalInt2`.

4.3 The Tank Block and Dynamic Holdup

The `Tank` block is the correct PulpMaster block for representing dynamic holdup in process vessels. It maintains a mass state vector (`Mass [i]`) for all dissolved components and integrates it at each time step:

$$M_i(t + \Delta t) = M_i(t) + \dot{m}_{i,\text{in}}(t) \cdot \Delta t \quad (4.1)$$

where M_i is the total mass of component i in the tank (kg), and $\dot{m}_{i,\text{in}}$ is the net mass flow rate (kg s^{-1}) of component i into the tank.

4.4 Xylan Verification Approach

4.4.1 Rationale for Using Xylan

As described in section 2.3.4, xylan is an ideal compositional tracer because its concentration in black liquor differs markedly between hardwood (≈ 12.5 g/kg) and softwood (≈ 2.8 g/kg) — a factor of approximately four. This large contrast makes it straightforward to detect the composition front as it passes through the evaporation plant. Xylan is also chemically stable under evaporation conditions, meaning its concentration at any downstream measurement point directly reflects the upstream cooking conditions at the time the liquor entered the system.

4.4.2 Laboratory Sampling Data

A laboratory sampling campaign was conducted at SCMS during a real HW \rightarrow SW \rightarrow HW transition. Black liquor samples were collected at regular intervals from the evaporation plant and analysed for carbohydrate composition — including xylan and glucomannan — using ion chromatography. The campaign produced 34 measurement points covering 228 hours (approximately 9.5 days) of transition, including both the come-up and come-down transients, that is, the rise and fall of the measured xylan concentration in the black liquor at the sampling point as the mill switches from SW to HW and back again (see figs. 4.1 and 6.1). This duration spans a full hardwood production campaign at SCMS, from the initial species switch through steady-state hardwood operation and back to the subsequent softwood switch. Analytical reproducibility was assessed from duplicate measurements of three samples, yielding a maximum replicate range of ± 125 mg/kg, which was adopted as the measurement uncertainty for all data points (Thorén & Parkås, 2025).

4.4.3 RTDB Operational Data

The SCMS Real-Time Database (RTDB) is an industrial process historian developed in collaboration with ABB, providing API access to continuously logged process measurements including tank levels, flow rates, temperatures, and dry solids content at sub-minute resolution. RTDB data from the sampling campaign period was used to set the initial conditions of the simulation (tank fill levels and feed flow rates), ensuring that the simulated transient corresponds to the actual plant state at the start of the transition. Data were filtered using average values and 90th-percentile estimates to capture representative operating conditions and suppress short-term noise from control actions and sensor fluctuations.

A key finding during model calibration was that using a fixed average flow rate was

insufficient to reproduce the measured xylan transient. Since flow rate directly affects both the hydraulic residence time of the storage tanks and the dry solids concentration in the evaporator, the time-varying WBL flow rate from the RTDB was implemented as a lookup table driving the simulation. This significantly improved agreement between the simulated and measured xylan profiles.

4.4.4 Model Comparison

Validation is performed by overlaying the simulated xylan concentration time series on the laboratory measurements and computing the root-mean-square error (RMSE) and mean absolute error (MAE) between the simulated profile and the 34 measurement points. The full comparison is presented in chapter 6.

4.5 Transition Optimization Scenarios

Four scenarios are investigated to identify strategies for reducing the wood species transition time and increasing the volume of on-specification prima product recovered per transition. The laboratory data from the sampled transition serves as the observed baseline against which each scenario is compared.

Two operational levers were identified as the primary variables for scenario analysis. First, the LM intermediate liquor storage tank represents the largest single holdup volume between the evaporator and the lignin separation feed; bypassing it directly reduces the volume of old-species liquor that must be displaced, and therefore hypothetically shortens the transition. Second, the LTJM4 recirculation stream returns partially concentrated liquor from Effect 2 back into the tank farm. A higher recirculation rate increases the dry solids content in the LTJM4 tank (which is operationally desirable for soap skimming) but simultaneously increases the effective hydraulic residence time of the tank farm, since more old-composition liquor is being cycled back rather than displaced forward. Varying the recirculation rate therefore trades off transition speed against soap-skimming performance.

Figure 4.1 shows the process layout relevant to the scenario definitions, identifying the locations of the LTJM4 recirculation tank, the LM1 intermediate liquor storage tank, the LM bypass, and the laboratory sampling point at the SBL tank outlet.

Theoretical minimum (S0): All intermediate black liquor tank volumes are set to 10 m^3 , effectively eliminating holdup in the tank farm. This represents the physically ideal lower bound on transition time.

LM tank bypass, 50% recirculation (S1): The LM intermediate storage tank is bypassed, reducing the effective holdup volume on the come-down transient. The

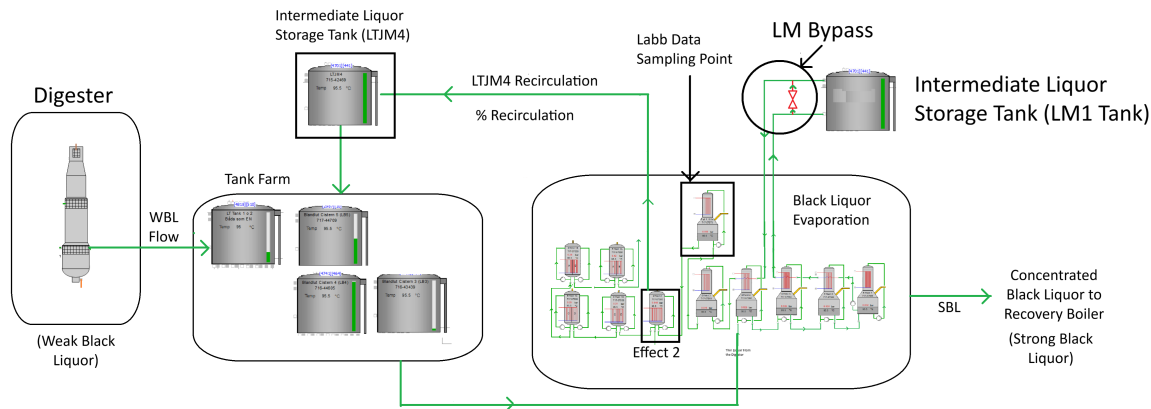


Figure 4.1: Simplified process schema showing the elements varied across the four scenarios. The LTJM4 tank (top left) receives a recirculation stream from Effect 2 at a controllable rate. The LM1 intermediate liquor storage tank (right, circled) can be bypassed, reducing the effective holdup volume between the evaporator and the lignin separation feed. The laboratory sampling point is located at the SBL tank outlet.

LTJM (mellantjock lut, medium-thick liquor) recirculation rate, a recirculation stream from Effect 2 back to the tank farm, is set to 50%. This scenario targets a faster come-down, meaning a quicker fall in xylan concentration as the mill switches from HW back to SW, thereby reducing the period of off-specification mixed lignin during the HW→SW switch.

LM tank bypass, 75% recirculation (S2): Same LM bypass configuration as S1 but with a higher recirculation rate of 75%. The higher recirculation rate increases the dry solids content in the LTJM tank, which is relevant for soap skimming, but results in a slower come-down transient compared to S1.

No LM bypass, 50% LTJM recirculation (S3): The LM tank remains in the flow path (no bypass), and the LTJM recirculation rate is set to 50%. This scenario introduces additional holdup on the come-up transient but allows the tank farm to buffer composition changes, showing the trade-off between come-up lag and operational stability.

4.6 Performance Metric

The primary performance metric is T_{95} : the time elapsed from the species switch until the xylan concentration at the laboratory sampling point (shown in fig. 4.1) reaches 95% of its new steady-state value. A reduction in T_{95} corresponds directly to a shorter period of off-specification mixed lignin. For the come-down transient, T_{80} (80% completion) is used as the reference since the simulation window does not extend far enough for all scenarios to reach 95%. The full simulation covers approximately

250 hours (900 000 seconds), capturing both the HW and SW transitions within a standard hardwood campaign at SCMS.

5 Model Development

5.1 Overview of the Existing SCMS ExtendSim Model

The SCMS ExtendSim model, developed using the PulpMaster library, provides an existing representation of the kraft pulp mill from wood chip feed through to the brown stock washing stages. The evaporation plant is not represented in the original model. The primary extensions developed in this thesis are:

1. Addition of HW/SW composition tracking via xylan (index 34) and glucomannan (index 35) parameters throughout all existing blocks.
2. Construction of a full 7-effect evaporation section with WBL and SBL storage tanks.
3. Calibration of all block parameters to match SCMS steady-state operating data.
4. Implementation of the HW→SW and SW→HW feedstock switching logic.
5. Inclusion of tie in connection to lignin separation plant.

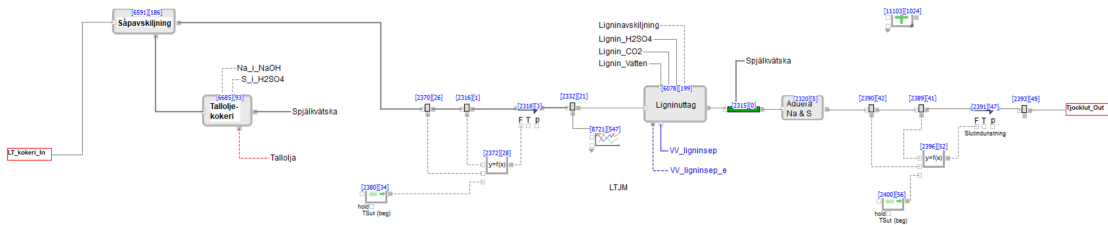


Figure 5.1: Base SCMS ExtendSim model prior to thesis extensions, showing the existing evaporation section with soap separation (Såpavskiljning), tall oil cooking (Talloiljekokeri), and lignin extraction (Ligninuttag) blocks. The 7-effect evaporator train was absent at project start.

5.2 HW/SW Composition Tracking Implementation

5.2.1 Xylan as HW/SW Marker

A first-principles kinetic model of xylan dissolution in the digester could in principle have been incorporated [18], but was not considered necessary for the purposes of this thesis. The timed injection approach is simpler to parameterise from available mill observations and is sufficient to reproduce the large-scale compositional dynamics of interest; accordingly, xylan is introduced via timed injections at the digester block.

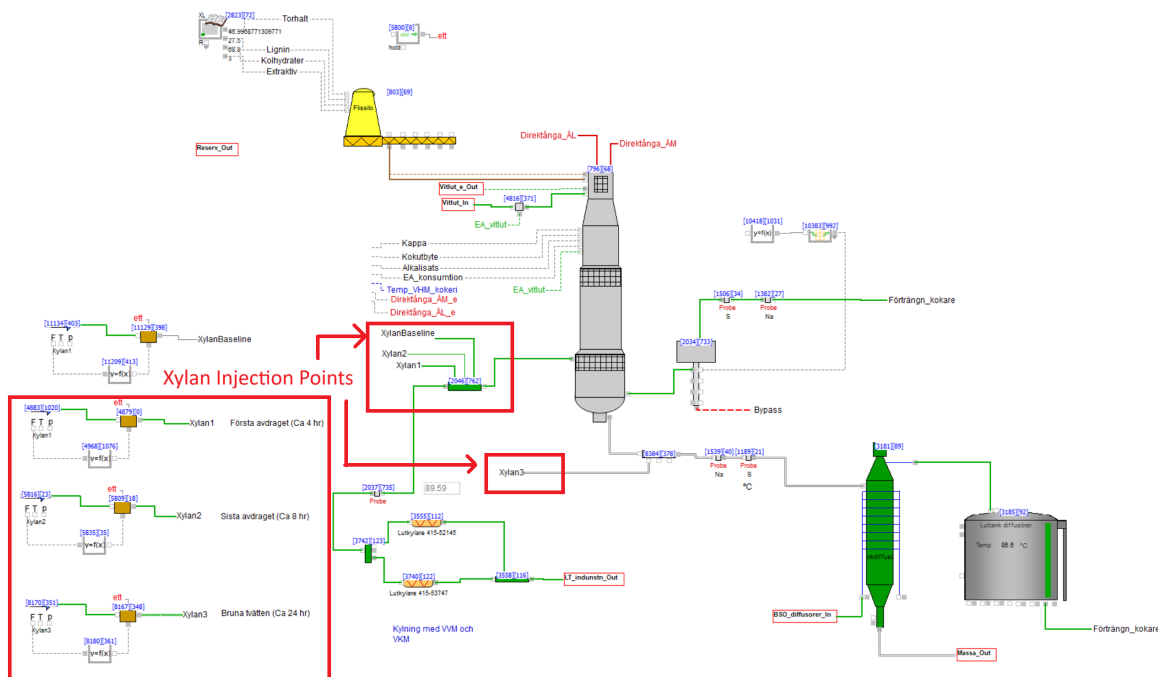


Figure 5.2: ExtendSim cooking section (Kokare block) showing the three timed xylan injection points: Xylan1 at $\tau = 4$ h (first screen), Xylan2 at $\tau = 8$ h (second screen), and Xylan3 at $\tau = 24$ h (brown stock washing outlet).

According to mill observations, the liquor extracted at the first digester screen (visible in fig. 3.2) becomes fully hardwood in character approximately 4 hours after the species switch; the second recirculation follows at 8 hours; and the brown stock washing plant completes its transition at approximately 24 hours. After 8 hours, the shortening of pulp fibre lengths also confirms the transition from softwood to hardwood pulp. These three time points define the xylan injection schedule (Xylan1, Xylan2, Xylan3); the injection concentrations were determined through trial and error and found to be approximately 1 g kg^{-1} wet liquor at each injection point. During the intermediate period (4–24 hours), the liquor entering the evaporation plant carries a mixed HW/SW composition. The model then tracks the hydraulic retention time through the black liquor holding tanks, whose volumes are significant and result in a further lag before the composition change propagates to the lignin separation feed.

5.3 Evaporation Section Construction

The evaporation section, including the tank farm, was built from scratch as the primary model contribution of this thesis. Tank farm vessels were parameterised using construction data for tank geometries and volumes, combined with RTDB data for average inter-tank flow rates and level indicators to set representative initial fill levels.

5.3.1 Model Architecture

Figure 5.3 shows the completed 7-effect evaporation model. Thin black liquor enters at Effect 7 and is concentrated progressively through to Effect 1, after which the strong black liquor feeds either the recovery boiler or the lignin separation plant.

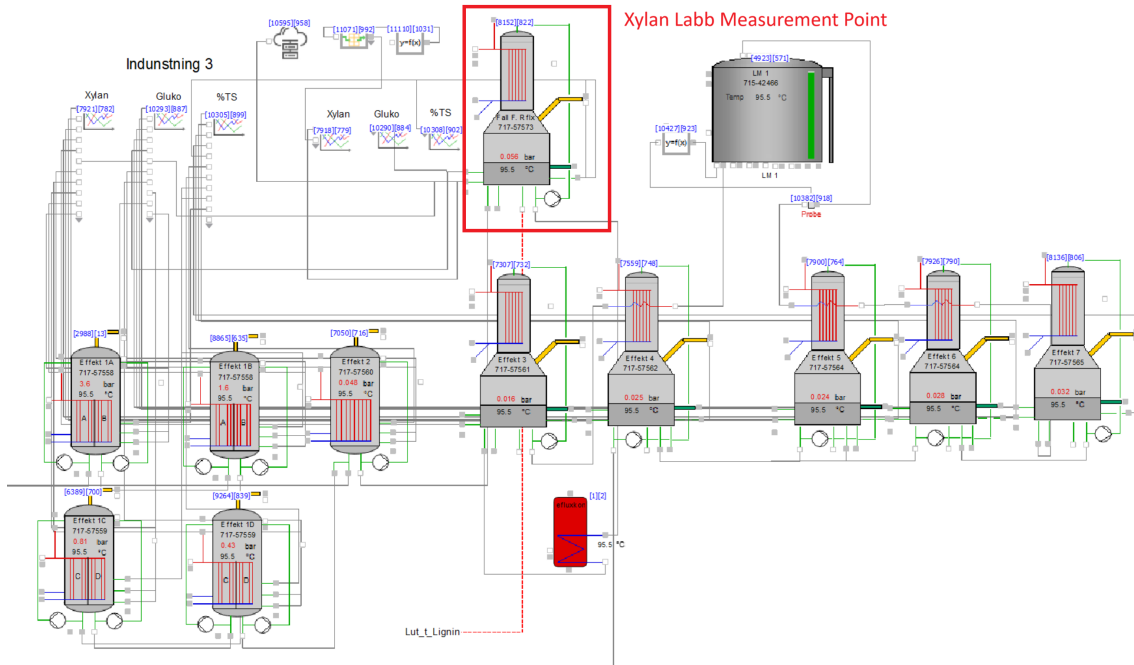


Figure 5.3: Constructed 7-effect falling-film evaporation model in ExtendSim (Indunsting 3). Thin black liquor enters from the right (Effect 7) and is concentrated progressively through to Effect 1 on the left. Xylan (Xylan) and glucomannan (Gluko) tracking are visible at the top left. The WBL storage tank (right, with level indicator) feeds the evaporator train.

5.3.2 Tank Farm Model

The tank farm model is shown in fig. 5.4. Each vessel is represented by a Tank block initialised with fill level and composition data from the RTDB at the start of the sampled transition. Initial xylan concentrations were set to HW steady-state values from the laboratory data.

5.4 Feedstock Switching Logic

Rather than modelling the digester kinetics explicitly, the species switch is represented by the three timed xylan injections described in section 5.2. At $t = 0$ the chip feed switches species; the xylan signal then steps up at 6 h, 8 h, and 24 h, reflecting the sequential arrival of the new-species liquor at the first screen, the second screen, and the washing plant outlet respectively. From $t = 24$ h onward, the liquor entering the evaporator tank farm is fully composed of the new species, and the model tracks

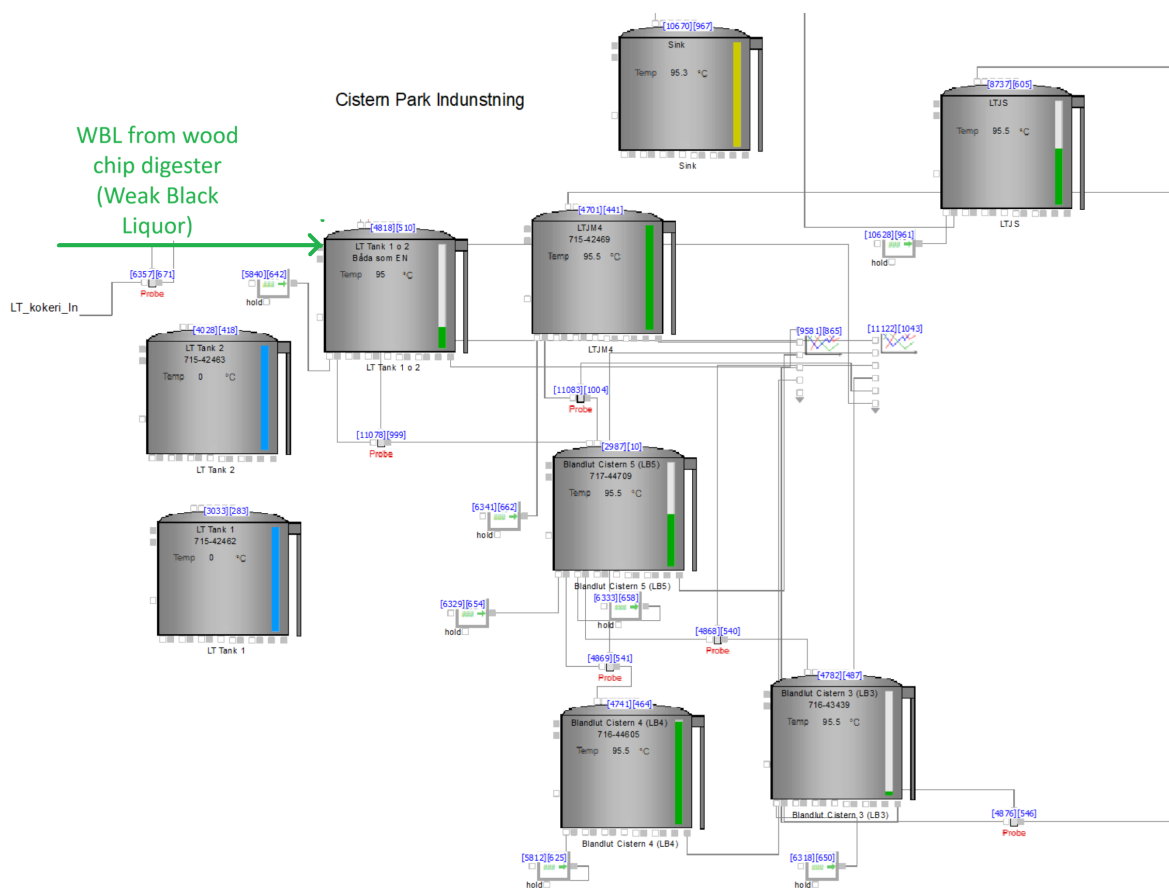


Figure 5.4: Extendsim tank farm model (Cistern Park Indunstning) showing the black liquor holding tanks upstream of the evaporator. LT Tank 1 and LT Tank 2 receive liquor from the digester; the Bandful Cistern tanks buffer flow between process sections. Tank fill levels and temperatures are visible for each vessel.

the subsequent displacement of old-composition liquor through the holding tanks and evaporator effects.

5.5 Model Assumptions and Simplifications

The following assumptions are made in the model:

1. **Perfect mixing:** All Tank blocks are modelled as perfectly mixed vessels (CSTR assumption). This approximation is considered reasonable for the weak black liquor storage tanks, where the relatively low dry solids content (approximately 15–20% DS) results in comparatively low liquor viscosity, supporting good bulk mixing. At higher dry solids content, such as in the intermediate and strong liquor tanks, viscosity increases and mixing may become less ideal. The validity of this assumption for each vessel is discussed in section 6.3; identifying tanks that exhibit systematic deviations from ideal mixing is an important direction for future model refinement.

2. **Quasi-static evaporator:** The `Industare` block does not maintain a dynamic mass state but propagates composition in pseudo-steady state at each time step. The liquor holdup within each evaporator effect is small compared to the storage tanks and its contribution to the composition transient is negligible.
3. **Time-varying flow rates:** WBL flow rates are driven by a lookup table of RTDB measurements from the sampling campaign rather than held constant, since flow rate directly affects hydraulic residence time and dry solids concentration.
4. **No xylan degradation:** Xylan is assumed to undergo no further degradation or reaction between the washing plant and the SBL tank. Evaporation temperatures are sufficiently low that additional peeling is negligible.
5. **No energy balance:** Heat losses and steam consumption are not modelled. Evaporation rates are set using design values calibrated to match the measured dry solids profile.

6 Results and Discussion

This chapter presents the simulation results for all four scenarios, compares them against the laboratory measurements, and analyses the contribution of individual tank farm vessels to the transition delay. Laboratory measurements carry an analytical uncertainty of ± 125 mg/kg (Thorén & Parkås, 2025); error bars are omitted from figures for clarity given the number of lines present.

6.1 Xylan Transient — Scenario Comparison

Figure 6.1 shows the simulated xylan concentration at the SBL tank outlet (lignin separation feed point) over the full 250-hour measurement period for all four scenarios, with laboratory data overlaid. The dotted vertical line at 186.4 h marks the SW species switch. Figures 6.2 and 6.3 show the come-up and come-down transients in detail. The best agreement with the laboratory data is obtained for the LM bypass, 75% recirculation scenario, confirming that the LM tank was bypassed during the sampling campaign. RMSE values are computed separately over the come-up transient (0–100 h, 17 measurement points) and the come-down transient (186–250 h, 13 measurement points); the HW steady-state plateau (100–186 h) is excluded from the error calculation as the plateau xylan value is a calibrated input to the model rather than a predicted quantity. The best scenario achieves a come-up RMSE of 1.00 g/kg and a come-down RMSE of 0.88 g/kg. Table 6.1 summarises the RMSE for all four scenarios.

Table 6.1: RMSE (g/kg wet liquor) for each scenario. S0: theoretical minimum (10 m³ tanks); S1: LM bypass, 50% recirk; S2: LM bypass, 75% recirk (best); S3: no LM bypass, 50% recirk. Overall RMSE over all 30 measurement points; come-up over 0–100 h (17 pts); come-down over 186–250 h (13 pts). HW plateau (100–186 h) excluded from all calculations.

Scenario	Overall RMSE (g/kg)	Come-up RMSE (g/kg)	Come-down RMSE (g/kg)
S0	2.20	1.93	2.76
S1	1.20	0.97	1.53
S3	1.07	1.43	0.45
S2	0.92	1.00	0.88

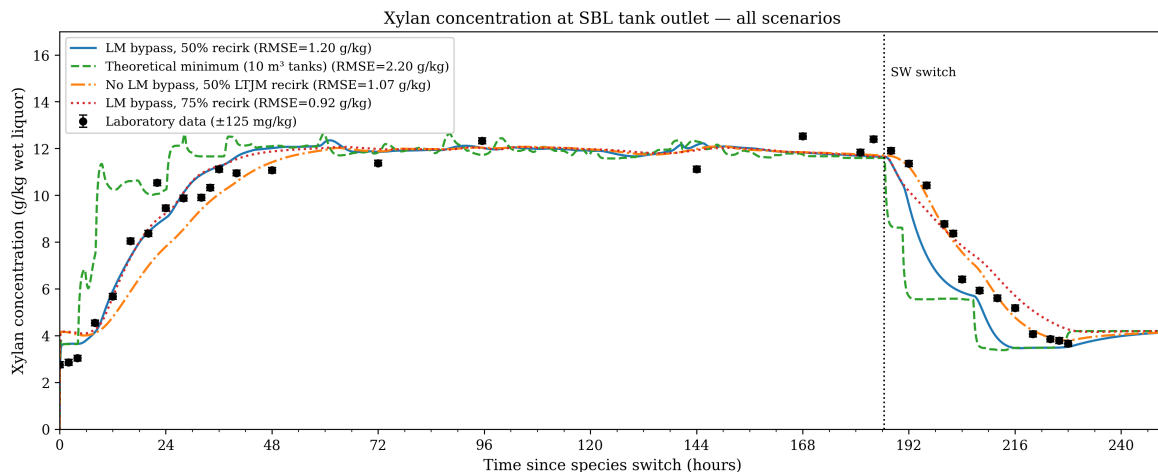


Figure 6.1: Simulated xylan concentration at the SBL tank outlet (lignin separation feed point) for all four scenarios, with laboratory measurements overlaid (black circles). The come-up transient (0–186.4 h) and come-down transient (186.4–250 h) correspond to the HW and SW species switches respectively.

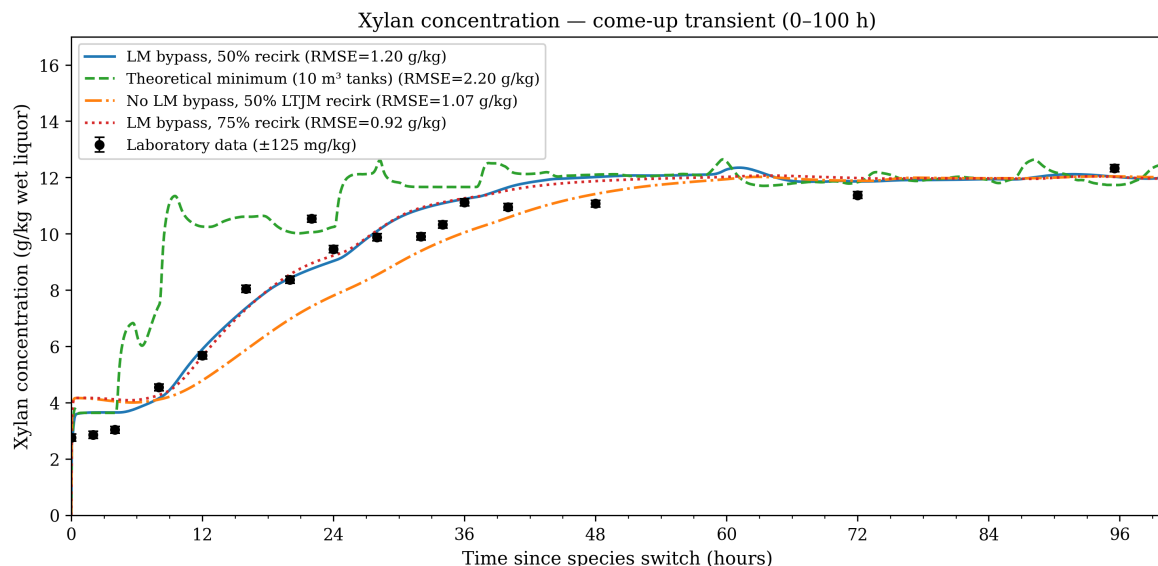


Figure 6.2: Xylan come-up transient (0–100 h) for all four scenarios with laboratory data. The theoretical minimum (green dashed) reaches $T_{95} = 25.3$ h; the LM bypass scenarios reach $T_{95} = 45.9$ – 55.3 h; the no-bypass scenario takes 60.9 h. The best-matching scenario (LM bypass, 75% recirk) achieves a come-up RMSE of 1.00 g/kg over the 17 measurement points in this window.

6.1.1 Interpretation of Scenario Results

The come-up results broadly matched expectations. Reducing tank holdup volumes to their theoretical minimum (S0) produced the fastest transition by a wide margin ($T_{95} = 25.3$ h), confirming that hydraulic residence time in the tank farm is the dominant bottleneck. This result was anticipated from the outset: less old-composition liquor to displace means a shorter transient, regardless of operating strategy. The LM bypass

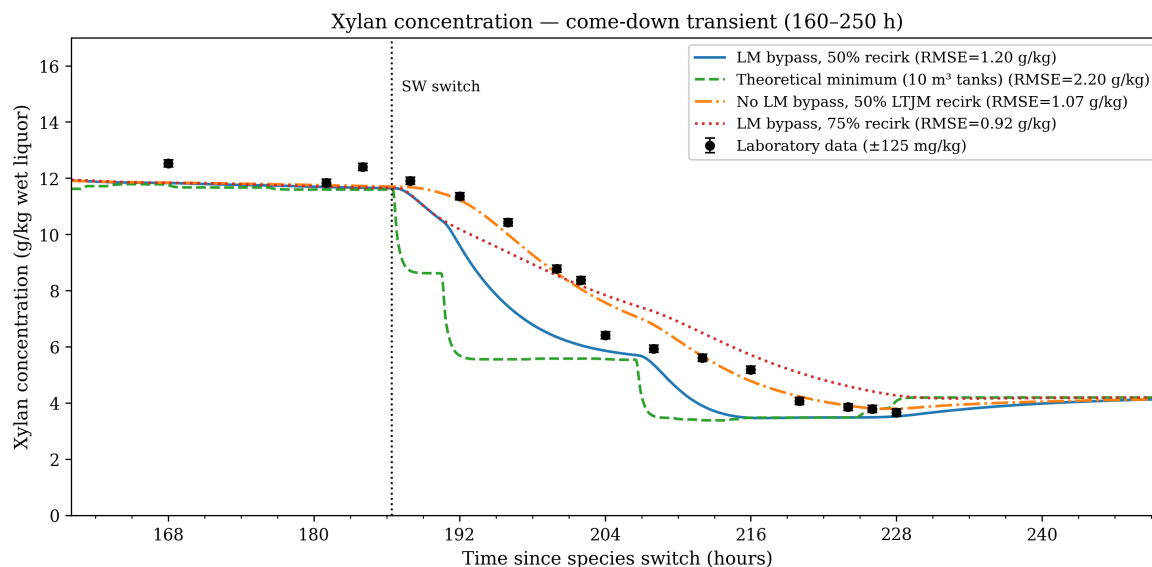


Figure 6.3: Xylan come-down transient (160–250 h) for all four scenarios with laboratory data. The LM bypass with 75% recirculation (red dotted) shows the slowest fall ($T_{80} = 36.7$ h), while the 50% recirculation scenario is considerably faster ($T_{80} = 23.1$ h after the SW switch). The best-matching scenario achieves a come-down RMSE of 0.88 g/kg over the 13 measurement points in this window.

scenarios (S1, S2) also behaved as expected, with the no-bypass scenario (S3) taking the longest at $T_{95} = 60.9$ h due to the additional holdup of the LM1 tank.

The come-down results were less intuitive than the tank holdup findings, and the effect of recirculation rate on transition speed was identified during model tuning rather than predicted in advance. The 50% recirculation scenario (S1) reached T_{80} in 23.1 h, considerably faster than the 75% scenario (S2) at 36.7 h. The physical explanation is straightforward once observed: at a lower recirculation rate, less liquor is diverted back into the tank farm, so more of the old-composition liquor is continuously bled forward and out of the evaporator train. A higher recirculation rate returns a greater fraction of liquor to the tank farm, slowing its displacement and prolonging the come-down transient. The recirculation rate therefore acts as a direct lever on how quickly old-composition liquor is expelled from the system.

6.2 Tank Farm Analysis

To understand which vessels dominate the transition delay, the xylan concentration and dry solids content were extracted for each tank farm vessel individually.

6.2.1 Dry Solids — Effect of Recirculation Rate

Figure 6.4 compares the dry solids content in three key tank farm vessels between the 50% and 75% recirculation rate scenarios. The LTJM4 tank operates in the range

44–52% DS, which is the zone where soap skimming occurs; a higher recirculation rate shifts the DS upward and broadens the period during which soap can be effectively skimmed.

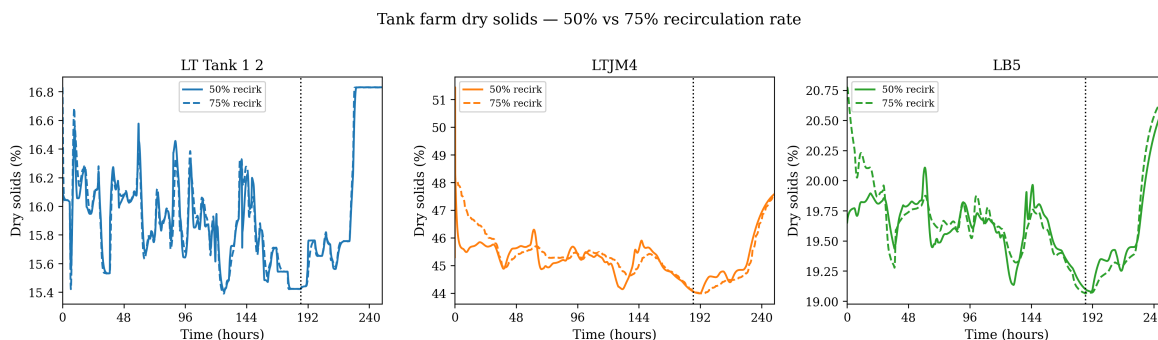


Figure 6.4: Dry solids content in the LT Tank 12, LTJM4, and LB5 vessels for the 50% (solid) and 75% (dashed) recirculation rate scenarios. The dotted vertical line marks the SW species switch at 186.4 h. LTJM4 operates in the soap-skimming range (44–52% DS); the higher recirculation rate elevates DS in this tank throughout the transition.

6.2.2 Holdup Contribution by Vessel

Figure 6.5 shows the xylan concentration in each tank farm vessel over the full transition period for the 50% recirculation scenario. The LM1 vessel (purple) exhibits the largest holdup lag on both the come-up and come-down, identifying it as the dominant contributor to the overall transition delay at the lignin separation feed point. The LB-series tanks respond faster, while LTJM4 occupies an intermediate position.

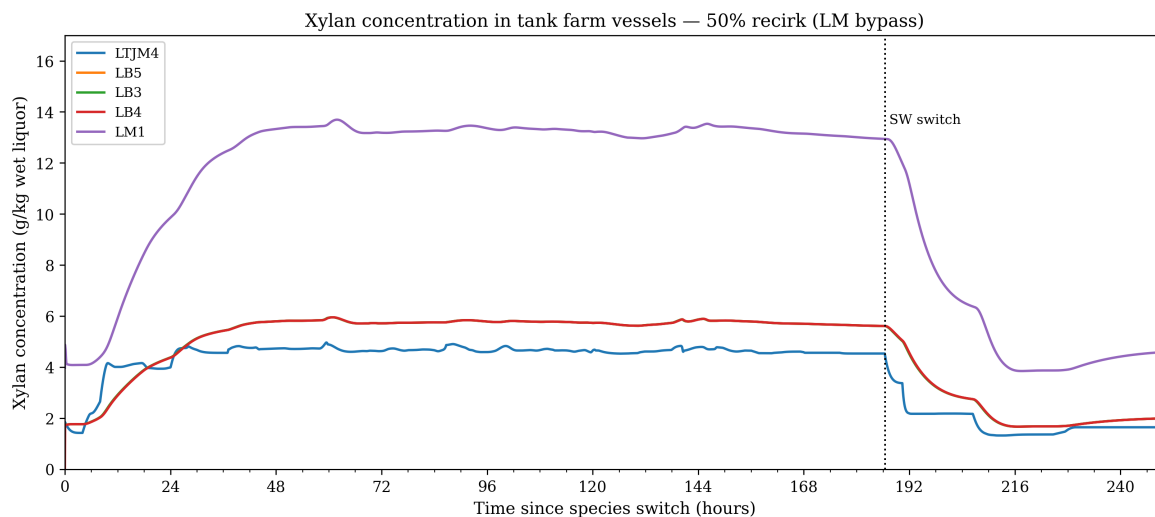


Figure 6.5: Xylan concentration in the five tank farm vessels for the 50% recirculation (LM bypass) scenario. LM1 shows the greatest holdup lag, rising last on the come-up and falling last on the come-down, making it the rate-limiting vessel for composition transitions at the lignin separation feed.

6.3 Discussion

6.3.1 Model Fidelity and Limitations

The CSTR assumption applied to all Tank blocks is a reasonable first-order approximation for well-agitated storage tanks, but real vessels exhibit channelling, thermal stratification, and short-circuit flow paths that redistribute residence times. Similarly, the constant flow rate assumption cannot capture the high-frequency fluctuations in pump rates, level controllers, and valve positions that are continuously present in an operating mill. These phenomena introduce noise-like deviations between simulation and measurement that no deterministic model can reproduce exactly, and they are a fundamental limitation of any lumped-parameter approach.

6.3.2 Calibration Methodology and Trial-and-Error Approach

A central challenge in this modelling work was that several key process parameters were not directly measurable from the RTDB. The recirculation flow rate to the LTJM4 tank, for example, could not be independently verified from available process instrumentation; the value used in the model was determined by iteratively adjusting the parameter until the simulated xylan transient matched the shape and timing observed in the laboratory data. This type of manual calibration is inherent to industrial process modelling when comprehensive flow measurement is unavailable.

Importantly, the objective of the calibration was not to achieve a minimum statistical residual against the laboratory data, but to produce a physically plausible model capable of reproducing the large-scale compositional phenomena — in particular the shape, timing, and magnitude of the come-up and come-down transients. The laboratory measurements served as reference signals for calibrating these dominant dynamics rather than as training targets for a curve-fitting exercise.

An early attempt was made to drive all inter-tank flows using raw time-series data from the RTDB for the entire duration of the transition. While this approach introduced realistic short-term variation into the simulation, it also introduced high-frequency noise into the xylan profiles that obscured the underlying compositional trend and made it difficult to distinguish the meaningful signal — the species composition front — from short-term process variability. Smoothed and time-averaged flow rates were therefore adopted, which preserved the dominant hydraulic behaviour while suppressing sub-hourly fluctuations that carry no useful information about the composition transient.

The xylan injection timing and magnitude at each of the three digester injection points also required iterative adjustment to reproduce the early-time rise observed in the laboratory data. Not all relevant inter-tank flow values were available from the RTDB,

and several parameters were assigned based on engineering judgement informed by operator interviews, with values refined until the simulated and observed transients agreed to an acceptable level. This trial-and-error character is an inherent feature of first-generation industrial simulation models, where the primary output is a working framework that can be progressively refined as more process measurements become available. A natural future step is to use this model to identify individual tanks whose simulated xylan profiles deviate systematically from measurements, which would indicate non-ideal mixing behaviour not captured by the CSTR assumption and would motivate a more detailed residence-time-distribution model for those vessels.

6.3.3 Generalizability

The modelling approach timed xylan injections combined with hydraulic residence time tracking through Tank blocks is generic and transferable to other kraft mills running dual-species operations or other lignin separation installations. The key mill-specific inputs are the tank volumes, fill levels at transition time, and the species-switch timing heuristics, all of which can be obtained from RTDB data and operator interviews.

6.3.4 Recirculation Rate and Downstream Dry Solids

One concern not addressed by the current model is the effect of recirculation rate on downstream dry solids content. The LTJM4 recirculation stream returns partially concentrated liquor from Effect 2 back to the tank farm, and a higher recirculation rate raises the average dry solids content of the liquor re-entering the evaporator. While this is captured qualitatively in the tank farm dry solids profiles (Section 6.2.1), the present model does not calculate evaporation rates from first principles and therefore cannot predict how the elevated dry solids propagates through each effect or whether it approaches the solubility limits associated with scaling and fouling on the heat transfer surfaces. Elevated dry solids in the higher effects could increase the risk of scaling, with potential consequences for heat transfer efficiency and equipment maintenance. This remains an open question that requires a model incorporating an energy balance and calculated evaporation rates to properly evaluate; this is identified as a priority for future development (see Section 7.4).

7 Conclusions and Future Work

7.1 Summary

This thesis developed and validated a dynamic process simulation model for Södra Cell Mönsterås (SCMS) using the ExtendSim platform and the PulpMaster block library. The model tracks the HW/SW lignin composition through the kraft pulp mill process chain from the digester through brown stock washing to a newly constructed 7-effect evaporation section, using xylan concentration as the primary compositional tracer. Xylan was injected at three timed points reflecting the digester transit delays (4 h, 8 h, and 24 h), and the model then resolves the hydraulic retention time through the black liquor holding tanks and evaporator train.

Model validation was performed against laboratory xylan measurements collected during a real HW→SW→HW transition at SCMS (34 sampling points over 228 hours). The best agreement was obtained for the LM tank bypass scenario with 75% recirculation. RMSE was evaluated separately over the come-up transient (0–100 h, 17 points) and the come-down transient (186–250 h, 13 points), excluding the HW steady-state plateau from the error calculation since the plateau xylan concentration is a calibrated model input rather than a predicted quantity. The best scenario achieves a come-up RMSE of **1.00 g/kg** and a come-down RMSE of **0.88 g/kg**, both within $\approx 9\text{--}10\%$ of the total xylan range of 9.7 g/kg. The model correctly reproduces the shape and timing of both transients. Residual deviations arise from two sources: (i) uncertainty in the initial tank fill levels and compositions at the time of the transition, which were estimated from RTDB data rather than directly measured; and (ii) the inherent limitations of the perfect-mixing (CSTR) assumption, which cannot capture the high-frequency flow fluctuations, level oscillations, and small-scale non-ideal mixing phenomena present in a real operating plant.

A key process observation emerged during validation: the plant was operating with the intermediate LM liquor tank **bypassed for maintenance** at the time of the sampling campaign. This was not known at the outset; the bypass was first identified through the model itself, when the simulated come-up transient consistently failed to match the measured xylan rise without it. The hypothesis was subsequently confirmed by cross-referencing RTDB data, which showed no active level signal for the LM1 tank; inspection of the bypass valve settings then confirmed the tank was out of service. Accounting for this bypass was essential to match the observed xylan dynamics. Quantita-

tively, the LM bypass reduces the come-up T_{95} (time to reach 95% of HW steady-state xylan) from 60.9 h (no bypass) to 45.9 h, a reduction of 15 h. On the come-down, the 50% recirculation bypass scenario reaches 80% completion in 23.1 h compared to 30.1 h without bypass. The scenarios that minimise tank holdup and reduce recirculation lag show the most significant shortening of the transition period, indicating clear potential to increase the volume of on-specification prima lignin product recovered per species switch.

7.2 Conclusions

The following conclusions are drawn from this work:

1. **Model validation:** The model was validated against 34 laboratory xylan measurements from a real HW→SW transition at SCMS. The best-matching scenario (LM bypass, 75% recirculation) achieved a come-up RMSE of **1.00 g/kg** and a come-down RMSE of **0.88 g/kg** (both ≈ 9 –10% of the 9.7 g/kg xylan range), evaluated over the transient periods separately from the steady-state plateau. Residual deviations are attributed to uncertainty in initial tank fill levels and the inability of the CSTR model to resolve high-frequency flow fluctuations present in real plant operations.
2. **LM tank bypass:** The plant was found to be operating with an intermediate liquor tank bypassed during the measurement campaign. Including this bypass in the model was essential for validation and represents a significant operational finding: the bypass reduces the come-up T_{95} by 15 h (from 60.9 h to 45.9 h) and accelerates the come-down.
3. **Dominant holdup vessel:** Analysis of the xylan concentration profiles across the tank farm shows that the LM1 vessel exhibits the greatest lag on both the come-up and come-down, identifying it as the rate-limiting vessel for composition transitions at the lignin separation feed point.
4. **Transition duration:** Under the LM bypass operating conditions that matched the sampled campaign, the come-up T_{95} is 45.9 h for 50% recirculation and 55.3 h for 75% recirculation. The theoretical minimum (10 m³ tanks) achieves $T_{95} = 25.3$ h.
5. **Model utility:** The verified model provides Södra with a practical digital tool for planning species transitions, training operators, and evaluating future process modifications without requiring physical trial-and-error at the mill.

7.3 Recommendations for SCMS Operations

Based on the simulation results, the following operational recommendations are made for Södra Cell Mönsterås:

- **Pre-transition tank drawdown:** Black liquor holding tank levels should be reduced to the minimum operationally safe fill level in advance of a planned wood species switch. The simulation results show this is the most effective single lever for reducing transition time, as the LM1 vessel was identified as the rate-limiting holdup volume.
- **LM tank bypass:** The current maintenance bypass of the intermediate LM liquor storage tank reduces the come-up T_{95} by approximately 15 hours compared to the non-bypass configuration. This bypass should be considered as a permanent operational strategy during species transitions, subject to operational safety review.
- **Recirculation rate:** A 50% recirculation rate on the LTJM tank provides a better balance between come-up speed ($T_{95} = 45.9$ h) and come-down speed ($T_{80} = 23.1$ h) than the 75% rate, which slows the come-down considerably.
- **Transition scheduling:** The model's predicted T_{95} value can be used by production planners to more accurately schedule the restart of lignin product acceptance, reducing the conservative buffer time currently applied.

7.4 Future Work

This thesis opens several avenues for future research and development:

Xylan vs. Lignin Transient Timing: This thesis uses xylan as a proxy for HW/SW lignin composition, but it is not yet known whether the xylan transient leads, lags, or coincides with the actual lignin concentration transient. If xylan responds earlier than lignin, it could serve as an early-warning indicator; if it lags, the lignin transition may be faster than the model predicts. Simultaneous measurements of both xylan and lignin during a transition campaign would resolve this question and potentially improve model accuracy.

Xylan Kinetic Model: Including a first-principles kinetic model of xylan dissolution and reprecipitation in the digester would replace the current timed-injection approach with a physically grounded description, improving early-time transient predictions.

Model Predictive Control (MPC): The transient model could serve as a plant

model within a model predictive control framework that actively manages tank levels and flow rates during species transitions to minimise mixed-species duration [14].

Inorganic Species Balance: Including sodium and sulphur concentration dynamics would allow research into scaling and fouling behaviour in the evaporator during transitions.

Energy Balance and Evaporation Rates: Including heat transfer correlations and calculated evaporation rates in the evaporator model would allow energy demand to be quantified as a function of liquor composition. Critically, this would also enable assessment of how the LTJM recirculation rate affects the dry solids profile across the evaporator effects, and whether elevated recirculation rates risk approaching scaling or fouling thresholds on the heat transfer surfaces (see Section 6.3.4).

Lignin Separation Plant Integration: Including the downstream lignin separation facility in the simulation would be a natural next step, providing a complete model from wood chip feed to dried lignin product.

Extended Scope: Including the bleaching plant and chemical recovery loop would enable a complete mill-wide assessment of the species transition effect.

Stochastic Transitions: Incorporating a realistic chip inventory depletion model in the digester feed would improve accuracy of early-time predictions, as real switches are not perfectly instantaneous.

Data Integration: Connecting the ExtendSim model to the RTDB API in real time would enable online state estimation and prediction of SBL composition without waiting for laboratory results.

Recovery Boiler Energy Predictions: Since the recovery boiler is the main steam producer, modelling the effect of lignin-lean black liquors on boiler load and electricity production would quantify the full economic impact of species transitions.

Xylan Extraction Plant: Xylan has applications across multiple industries; this model provides the upstream process foundation for designing a future xylan extraction facility at SCMS.

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A Gantt Chart and Project Timeline

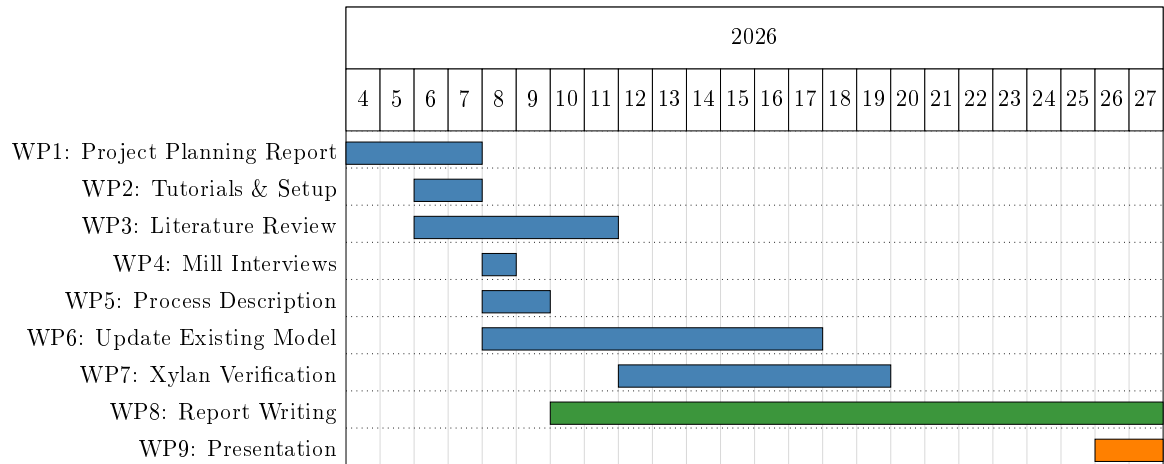


Figure A.1: Project timeline (Gantt chart) from Week 4 to Week 27, 2026.