Meeting 4

Date	Tuesday, 02 February 2021
Attendees	Dr Ali Yetisen (AY), Marie Jones (MJ), Mathusan Kandiah (MK), Zong Lee (ZL), Yuxin Liu (YL), Mustafa Nasar (MN), Helen Ogbobi (HO), Wei Ooi (WO), Andreas Richardson (AR), Stephen Tan (SN), Sathurthini Thurairatnam (ST), Mingchuan Zheng (MZ), Antonia Feilden (AF), Abdullah Ahmed (AA)
Apologies	None
Chair	Mingchuan Zheng (MZ)
Secretary	Marie Jones (MJ)

Minutes

Item	Discussion
1 – Implementation of last meeting suggestions	MZ: set availability table, PowerPoint for daily checks → better group coordination. All: no comment
2 – Progress update	**Synthesis and Reactor teams** MZ: collaboration with reactor team, completed design for nitration of toluene and o-toluidine synthesis. Bottleneck: oxidation of nitrotoluene to nitro-benzaldehyde ZL: challenge is to collect useful kinetic data → how do we work around that if we can't get useful data? AY: 3 approaches 1) educated guess, look at similar product from same market, do we have any comparable products from the industry? MZ: no kinetic data for intermediate step to benzaldehyde → only data for nitrotoluene directly to benzoic acid AY: have you explored simulation packages so far and what was the outcome? MZ: we haven't done simulation yet, from Aspen expert → do estimation with aspen, we don't need comprehensive set of kinetics data for interim report (conversion vs time might sufficient) AY: comments from expert? YL: common to not find kinetic data in industry → only use yield and conversion to simplify but if we want to fully design the reactor, we need the intrinsic rate of reaction, for interim we only need conversion value. AY: what did expert advise you to do? YL: all literature gives conversion vs time → get concentration profile → chose reaction time and extrapolate. AY: You can make extrapolation that is perfectly fine to do extrapolation but determine error from extrapolation. How would you do extrapolation actually? YL: R^2 analysis on Matlab or Excel AY: Good start but what if it is not linear? MZ: assume first order so should be linear. AY: if more complicated kinetic, R^2 should be close to 99% → we send him error

AF: Have you consider reduction and then oxidation?
AR: reduction and then oxidation → oxidation attacks amino group →takes you back to where you started ➔ it is preferred to do oxidation followed by reduction.
AF: have we started looking at SDS of product?
AR: broadly considering it, when we see very hazardous chemicals → consider factor as we go along.
HO: we have NFPA values, auto-ignition temperature, flash point
MJ: What are the 3 other approaches to find kinetics?
AY: 2) Info from publication, patents
What do you get from patents and papers → say it's close enough from our work, comparable studies, extrapolate that data and cite in report
AY: extract the data we need from those studies
AR: usual problem is that they only give partial info, kinetic constant but not activation energy
AY: make sure data from two papers are compatible if we put them together
AY: 3) reach out to alumni in industry + email expert frequently
MZ: no success in reaching out so far
AY: verify and validate that result are reasonable → very important
AF: look at supplementary info of paper + email authors
MZ: people usually don't respond
AY: not motivated to reply to undergrads
AR: papers from 70s, are people even still around?

ZL: question reactor: for interim report, are you looking at high level like PFR/CSTR or details for microreactors?
AY: details not so important in first report → have correct direction, don't go too much in detail but we still need to have equal distribution of different sections → don't do 60% of report on synthesis → balance between details and general → use space accordingly and use small figures like in papers, he prefers short reports

MJ: should we not consider sections weighting in Klaus' assessment form for size of sections?
AY: arrange like that too → find with both approaches but more words don't always mean higher grade

Separation team
MK: nitric acid recovery, decanter on aspen → we use calculator block → suggestion for Aspen expert; nitrotoluene separation, plan to have most of it done in the next two days, might be too optimistic
AY: how are you including modularity?
MZ: modularity comes form ability to switch between production of aminobenzaldehyde and aminobenzoic acid. Change residence time by changing reactor volume → multiple reactors with by-passes.
AY: to recap, modularity can be applied to type of chemicals, volume produced, purity → look at Merck, sigma-aldrich for different purity → don't always need highest purity level → be able to switch for specification of customer
MK: we can play with purity levels

SN: downstream depends on reaction conditions for oxidation and hydrogenation

If low conversion, recycle valuable feed
Include modularity → range of purity → we will consider
Question to AY: besides stream table and H&M balances for separation units + quick sizing, what else to include in interim report?
AY: most important → evidence-based approach → present data and assumptions of each separation step
YL: separation first part → patent search → good info on isomer separation → been following that so far
AY: make sure you have validation step, back it up with data and publication but justify why we chose this options among all the alternations, produce our know data (bunch of graphs → make more clear decision)
MK: Jackland analysis → look at physical data and safety
AY: very good to have in decision process!

Aspen Modelling
YL: presentation of flowsheet: 1) toluene nitration → 99% conversion in small reactor → consider microreactor, 2) decanter replaced by distillation → aspen model doesn't have to be perfect, as long as literature backs it up → consider replacing B1 with calculator block 3) B3 distillation for ortho/para-isomers
AY: too technical, just give general overview and issues, don't discuss details, should be done with technical experts

EHS team
HO: wrote sections, did table for hazard identification, working on risk matrix, identified main hazards but hard to rank → check with Chris how to do that without too much subjectivity from own judgement, doing F&EI for nitration → problem with pressure relief → ask Chris, we need to do waste treatment, waiting for other people
AY: Chris comments on safety?
HO: talked about expectations of interim → consider safety and environment in decision making steps for plant design

Economics team
MN: excel for CAPEX estimations and EP1, Bridgewater method for CAPEX calculation, writing market analysis
ST: market analysis, do we need to explain assumption for demand value in report?
AY: yes include market, who will be our main customers?
ST: pharma and agrochemicals
AY: name of companies, where are they and what are they selling as end products?
ST: we don't know that level of details
AY: Target customer companies, example with GSK → look at product portfolio and what do they need to produce that, who are the competitors, purity, volumes sold, suppliers
High level overview of what companies are doing → based on main products → look at market trends → estimation production range
ST; looking at market report so far
AY: look up 2-3 companies in China, find suppliers
SN: do you have a data base/website to recommend?
AY: simple Google search, can someone quickly look for supplier in china, do it live

	MZ: found shanghai chemex group AY: easy to find suppliers/competitor/volumes
3 – Expectations for interim report	MZ: what do you expect from us in interim report? AY: Have abstract overview, overall summary of 200 words Intro Process synthesis Process description Sizing One page discussion before conclusion→ regarding assumptions made, results obtained → compare our own work to published work, limitations, how we are moving forward with main report Are you writing in Latex? SN: in Latex AY: Antonia, Abdullah's comment on report structure AA: even distribution because interim report AY: only provides guideline and Klaus decides on final grade AF: need to more time to give meaning full feedback → good to have chemistry, process, economics, EHS AA: referencing of literature → kinetics AF: if we have space, product purity, ex: methanol market for different purity, add economics justification in synthesis, purer more expansive
4 – AOB	AY: keep it high level, just say in which direction we are going Something on AF and AA Offers to give feedback on interim report before AY: timeline, send 3 days in advance, increased responsibility (family, coursework, etc), not available on short notice, doesn't include weekends (lol), get to AF and AA by Friday, get feedback during the weekend → exception for this time because tight schedule AF and AA: OK to have a look over the week-end → send on Friday AY: copy him in email
5 – Finishing	**Next meeting: 13:00 Tuesday 9 February 2021.**

Actions

Description	**Assignee**	**Due (18:00)**
Send interim report draft to AF, AA, AY	All	05/02
Synthesis		
- Complete kinetics model to level of interim report requirements	AR, MJ, MZ, ZL, WO	03/02
- Finalise routes for 4-aminobenzoic acid and 4-aminobenzaldehyde	AR, MJ, MZ, ZL, WO	03/02
- Give conversion data of all reactions	MJ	03/02
Reactor		
- Sizing of reactors	AR, ZL, WO	05/02

- Qualitative design of nitration reactor	AR, ZL, WO	05/02
- Exploration of reactor alternatives	AR, ZL, WO	05/02
Separation		
- Finalise technique for each separation step	MK, SN	03/02
- Get mass and energy balances for each separation	MK, SN, YL	04/02
- Sizing of units	MK, SN, MJ	04/02
Aspen Modelling		
- Model oxidation and hydrogenation reactions	YL, MJ, MZ, AR, ZL	04/02
- Model downstream processing	YL, MK, SN	05/02
- PFD	AR, MJ	06/02
Business		
- Revise market analysis	ST	04/02
- CAPEX estimation	MN, ST	
- EP1	MN, ST	
Safety		
- consult Chris at next EHS concerning Fire and Explosion Index and ranking likelihood and severity for risk matrix	HO, ST, AR, MJ, MZ, ZL, WO	04/02
- Talk to synthesis/reactor/flowsheet team about pathways considered to ensure inherently safer design is implemented	HO, ST, AR, MJ, MZ, ZL, WO	05/02

Approval

Ali K. Yetisen	Mingchuan Zheng	
Dr Ali Yetisen *Facilitator*	Mingchuan Zheng *Chair*	Marie Jones *Secretary*

Signature: Mingchuan Zheng (Feb 2, 2021 16:21 GMT)

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Final Audit Report 2021-02-02

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