#### Diary Bullet Points and Information:

# Week 1 - January 6th to 10th

- Training
  - o HR stuff
  - Understanding the company
  - Meeting interns
  - o Engineering skills
  - o Analysis skills
  - Lab practical work
  - JMP and stats training

# Week 2 - January 13th to 17th

- Training & Ansys Fluent Upskilling
  - o Ansys first time
  - Working in SpaceClaim
  - o Development of different models
    - Vortex simulations
    - Filtration systems
    - VOF to DPM
    - Particle tracking
- Meeting with supervisor regarding work and potential areas to go into
  - o Previous experience in modelling
  - Work in the max planck
  - o Discussion of what to do
    - RStudio work on the WebApps
    - Python Work with CFD engineer for the improvement of processes
    - Modelling with Ansys
    - Modelling with SpaceClaim

### Week 3 - January 20th to 24th

- Ansys Fluent and R Upskilling
  - o VOF to DPM work
  - o Improving Documentation that exists
  - o Addition of new tutorials
- R Upskilling
  - Analysis of the WebApps

## Week 4 - January 27th to 31st

- Modelling Tech Updates
  - o Brining Plotly into use in the company over Esquisse

- Beginning of the WebApp Auditing
  - Working on Large and Small molecule upscaling
  - Centrifugation
  - o Cores of Shiny and RStudio

### Week 5 - February 3rd to 7th

- Building model for the OptiMax reactor parts
  - Determining the pitch
  - o Number of turns
  - Screw dimensions
- Continuing webapp auditing
  - Finishing Large and Small molecule upscaling fixed issue with reactivity by improving requirements, focus on renaming the variables and improving the documentation for explanations
  - Building a script for automatic email systems using Microsoft365R and sendmailR – ultimately failed due to SMTP security concerns

## Week 6 - February 10th to 14th

- Continuing the Ansys fluent documentation and assisting with a fluent problem to do with a syringe pump and fluctuating pressures in a system by moving the inlet in the reactor
- Building an animation creator to convert JPEGs and PNGs from Ansys fluent to .mp4 formats using offline systems and bypassing FFMEPG dependencies
- Building a wordcloud generator for the "BeYou" team to which can identify synonyms and group words together to assist with International Womens Day activities

#### Week 7 – February 17th to 21st

- Grandmother died so wasn't in work

Week 8 - February 24th to 28th

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Week 9 - March 3rd to March 7th

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## Week 10 - 10th March to 14th March

- Continued the WebApp Audit
  - Finished Plaque assay
  - o NTA
  - o Equivalence testing

- Redoing the printing chemistry equipment via Ansys to ensure correct configurations for the printing process

#### Week 11 - 17<sup>th</sup> March to 21<sup>st</sup> March

- Development of the Bayesian Optimisation DOE concept
- Foundations of the WebApp for Bayesian
- Manging Conda environments, YML files, GitHub cloning
- Testing of the Bayesian Concepts for DOE
  - Major reductions in experiments
  - o Improvements in computation time
  - Development of test cases
- Opening up to advanced signal deconvolution using machine learning techniques
- Finalising the model for printing the chemistry equipment and beginning the printing process with an exterior company

#### Week 12- 24th March to 28th March

- Presenting the Bayesian Optimisation App
- Beginning upscaling project for client with the development of Geometry, having kick off meetings and developing the simulation plans
- Improving the application of the Bayesian Optimisation, opening up to new surrogate and acquisition models, potential for moving into Fourier transform based models
- Researching into automating GC-MS using neural networks couple with NIST libraries and advanced signal deconvolution techniques
- NIBRT career fair

#### Week 13 - 31st March to April 4th

- Finishing Bayesian Optimisation App and troubleshooting designs
- Testing Multi Optimisation for CFD grid designs and applications
- Developing benchmarks for analysis of Bayesian model configuration for different applications
- Richardsons extrapolation for CFD analysis with Bayesian model
- Running CFD for velocity contours, Vortex analysis and COV mixing time determinations