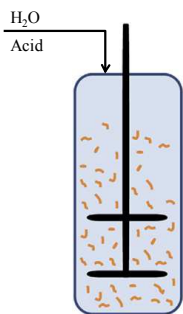


## 1. Pectin Extraction Process

Extraction by acidic hydrolysis from peels of citrus fruits

- Batch operation with several tanks
- The pectin quality can be characterized by intrinsic viscosity (IV) and degree of esterification (%DE)
- Process conditions (Temperature and pH) and proportions of peel/solvent vary within a limited range which is known to result in a desired particular KPI profile

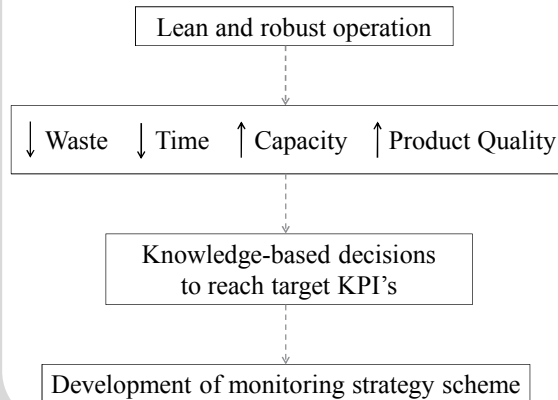


### Key Performance Indicators:

- IV
- %DE
- $C_{\text{pectin,bulk}}$

## 2. Objective and Motivation

From recipe-driven to a model-based approach



## 3. Dynamic Modelling

First principle model describing the non-linear process in respect to the KPI

- Prediction of the desired KPI
- Flexible applicability over a wide operational range of T & pH
- Central role in model-based approaches
  - Process understanding
  - Troubleshooting
  - Monitoring
  - Continuous process optimization

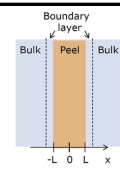
$$\frac{\partial c_{\text{pectin(peel)}}(t, x)}{\partial t} = D_{\text{pectin}} \frac{\partial^2 c_{\text{pectin(peel)}}(t, x)}{\partial x^2} + k_{\text{hydrolysis}} \cdot c_{\text{pectin(peel)}}(t, x)$$

$$\frac{\partial c_{\text{protopectin(peel)}}(t, x)}{\partial t} = -k_{\text{hydrolysis}} \cdot c_{\text{pectin(peel)}}(t, x)$$

$$\frac{\partial c_{\text{pectin(bulk)}}(t, L)}{\partial t} = \frac{A_{\text{total}} \cdot k_{\text{masstransfer}}}{V_{\text{total}}} \cdot (c_{\text{pectin(peel)}}(t, L) - c_{\text{pectin(bulk)}}(t, L)) - k_{\text{degradation}} \cdot c_{\text{pectin(bulk)}}(t, L)$$

$$\frac{\partial c_{\text{estergroup}}(t, L)}{\partial t} = DE_0 \cdot f_{GA} \frac{A_{\text{total}} \cdot k_{\text{masstransfer}}}{V_{\text{total}}} \cdot (c_{\text{pectin(peel)}}(t, L) - c_{\text{pectin(bulk)}}(t, L)) - k_{\text{de-esterification}} \cdot c_{\text{estergroup}}(t, L)$$

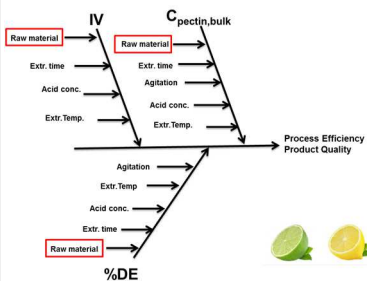
$$IV = IV_0 \cdot \exp(-k_{IV} \cdot t)$$



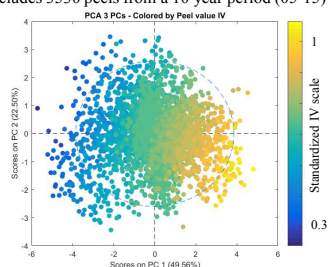
Development based on fundamental physical phenomena and a parameter training set: •Pilot scale •T vs pH DoE •one peel type

## 4. Identified Problems

### ➢ Lack flexibility for different peels

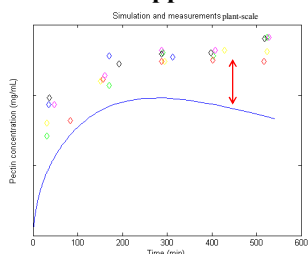


Preliminary exploratory analysis of historical dataset includes 3530 peels from a 10 year period (05-15)



Parameters that are inherently different from peel-to-peel are fixed or estimated for the training peel → Unaccounted uncertainty propagating into the output uncertainty

### ➢ Cross-scale application issues

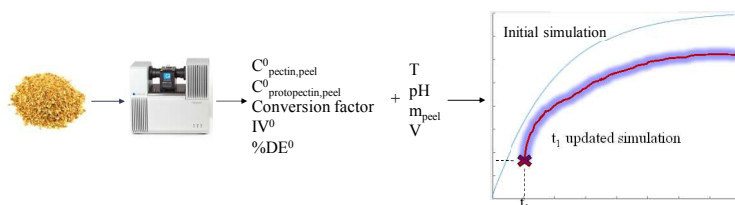


Sensitive parameters estimated at a different scale of application:

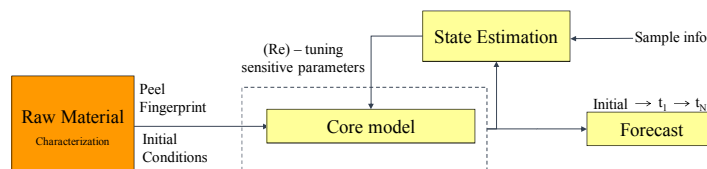
- Model alteration
- Re-tuning of parameters
- Hybrid approaches

## 5. Monitoring Strategy

Flexible model scheme that copes with raw material discrepancies by providing better initialization parameters for each different peel that arrives at the process line



Combination of state-of-the-art state estimation algorithms together with chemometric techniques to provide the process operators with a decision making tool for process optimization



## 6. References

The 1<sup>st</sup> principle model used in this research was developed in :  
 N.M. Andersen, T. Cognet, P.A. Santacoloma, J. Larsen, I. Armagan, F.H. Larsen, K.V. Gernaey, J. Abildskov, J.K. Huusom, Dynamic modelling of pectin extraction describing yield and functional characteristics, Journal of Food Engineering, Volume 192, January 2017, Pages 61-71