Deterministic and Stochastic Optimal Control of a Batch Cooling Crystallizer

Tushar Gupta (13CH30023)
Guide : Prof. Debasis Sarkar

Overview

Importance

- The batch system helps to obtain a narrower **Particle size distribution (PSD)** with high crystal purity.
- Finding effective control strategy to obtain a desired CSD is significant in order for improving the performance of batch crystallization processes

Objective

- The project aims to obtain optimal control analysis of batch crystallization process characterized by determination of the time varying profiles.

Concepts

- Deterministic Control using Maximum Principle Formulation.
- Propagation of Uncertainties through Stochastic **Ito Processes** and **Polynomial Chaos Expansions**.

Contents

- Model Formulation
- Deterministic Optimal Control
- Uncertainty Quantification
  - Ito Processes
  - Polynomial Chaos Expansions
- Application to Unseeded Crystallization Process

Essentials for Control Strategy

- The main control parameters affecting crystallization are **Temperature** and **Supersaturation**.

$$\text{Supersaturation} = \Delta C = C - C_s$$

$$\text{Relative supersaturation} = S = \frac{\Delta C}{C_s}$$

- Crystallization occurs through the following main phenomena :
  a. Nucleation
  b. Crystal Growth
  c. Agglomeration
  d. Breakage

- It is essential to be incorporate the above kinetics accurately to build a precise computational model.

Model Formulation

Modelling Batch Crystallization

- **Population Balance equations**
  - Modeling of a batch crystallizer involves the use of population balances to model the **crystal size distribution**.

$$\frac{\partial n(r,t)}{\partial t} + \frac{\partial G(r,t)n(r,t)}{\partial r} = B$$

- **<u>Moment Model for reduction of Population Balance Equations to O.D.E</u>**

$$\mu_i = \int_0^{\infty} r^i n(r,\,t)\,\mathrm{d}r$$

$$\mu_i^{\,\mathrm{n}} = \int_0^{r_g} r^i n(r,\,t)\,\mathrm{d}r$$

$$\mu_i^{\,\mathrm{s}} = \int_{r_g}^{\infty} r^i n(r,\,t)\,\mathrm{d}r$$

- The subscript i indicates the order of the corresponding moment.

- **Definition :**

$$\mu_0^s = \text{constant} \qquad \frac{d\mu_0^n}{dt} = B(t)$$

$$\frac{d\mu_i^s}{dt} = iG(t)\mu_{i-1}^s(t) \qquad i = 1, 2, 3 \qquad \frac{d\mu_i^n}{dt} = iG(t)\mu_{i-1}^n(t) \qquad i = 1, 2, 3$$

- Fourth-order moments and higher do not affect third-order moments and lower, implying that only the first four moments and concentration can adequately represent the crystallization dynamics .

- Thus, State variables are defined as :

$$y_i = [C \quad \mu_0^s \quad \mu_1^s \quad \mu_2^s \quad \mu_3^s \quad \mu_0^n \quad \mu_1^n \quad \mu_2^n \quad \mu_3^n]$$

where, $\frac{dC}{dt} = -3\rho k_v G(t)\mu_2(t)$

Deterministic Optimal Control

Problem Definition

- **Aim** : find an optimal temperature trajectory, which minimizes the total volume of fine crystals, and maximizes the size of seeded crystals in order to satisfy the product quality requirements.

- **Objective Function** :

$$\max_{T(t)}\{\mu_3^{s}(t_f) - \mu_3^{n}(t_f)\}$$

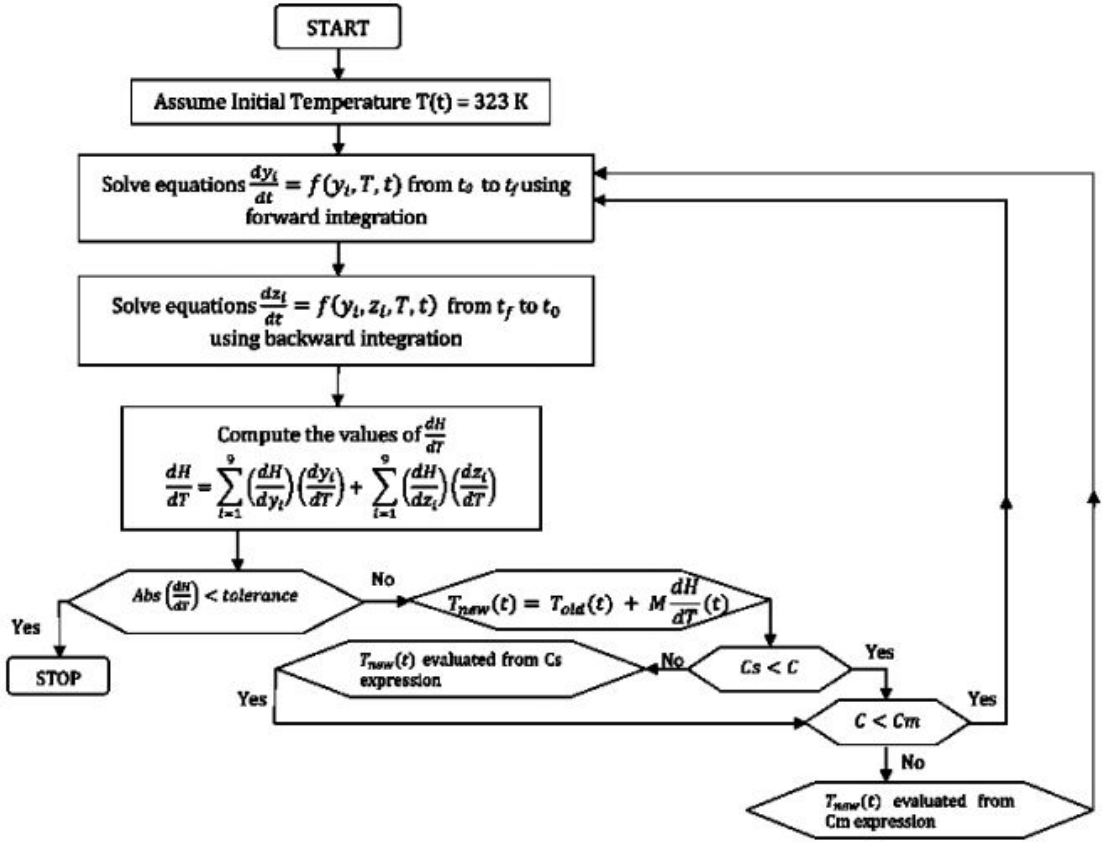
- **Active Constraints (**maintains the supersaturation condition**) :**

$$C_s \leq C \leq C_m$$

- A **Maximum Principle** formulation is used where Hamiltonian takes an extreme value for the control variable at each control point.

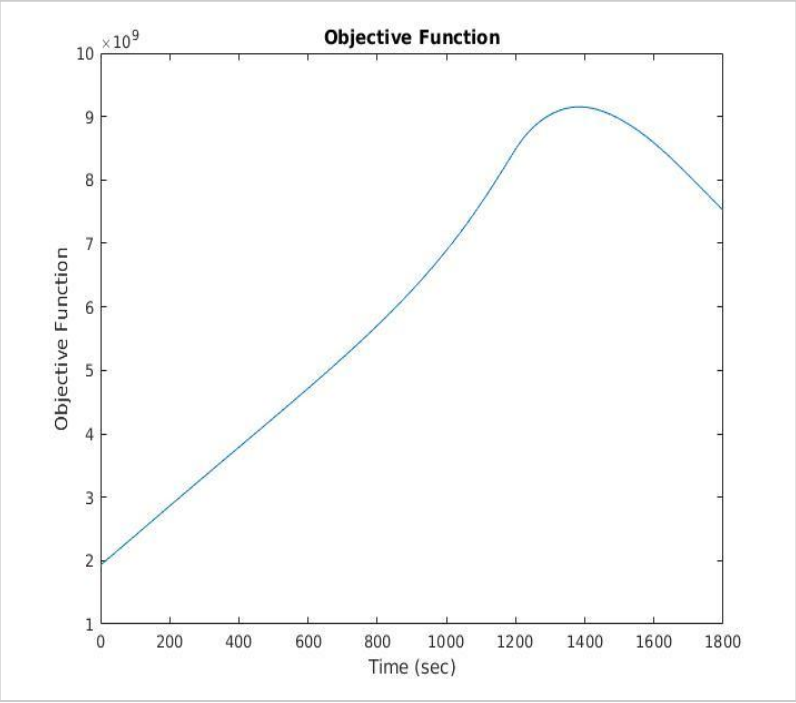
$$T^{new}(t) = T^{old}(t) + M\left(\frac{dH}{dT}\right)$$

Algorithm



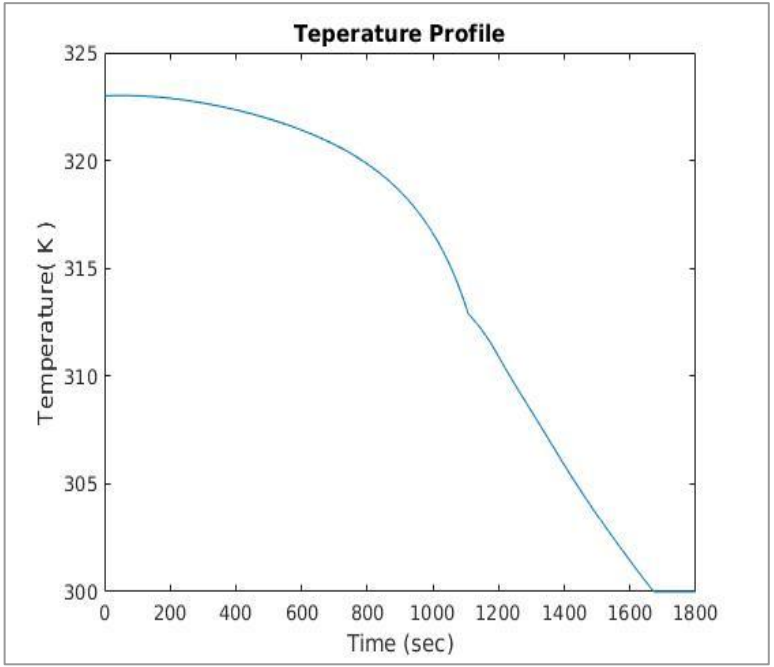
Overall Flowchart
Image Source : Yenkie et al.

Results



- Objective function reaches a peak value of 9.153 X 10^9 at t = 1387s which is the required aim of the modelling.
- The modelling has been done for potassium sulphate crystals
- Various methods of integrating ordinary differential equations were experimented upon during the implementation in **Python** and **Matlab**

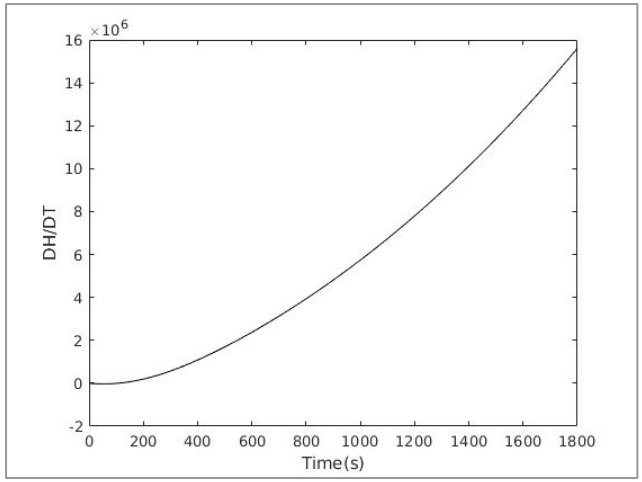
Results



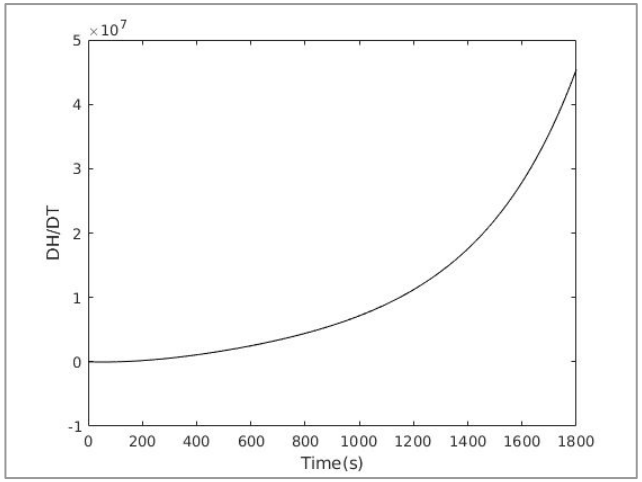
- This cooling profile is obtained for the final iteration.
- The initial temperature here is 323 K which gets reduced to 300 K.
- Remains at a steady value after reaching that point.

Results

- The value of the Hamiltonian derivative is shown after each iteration :

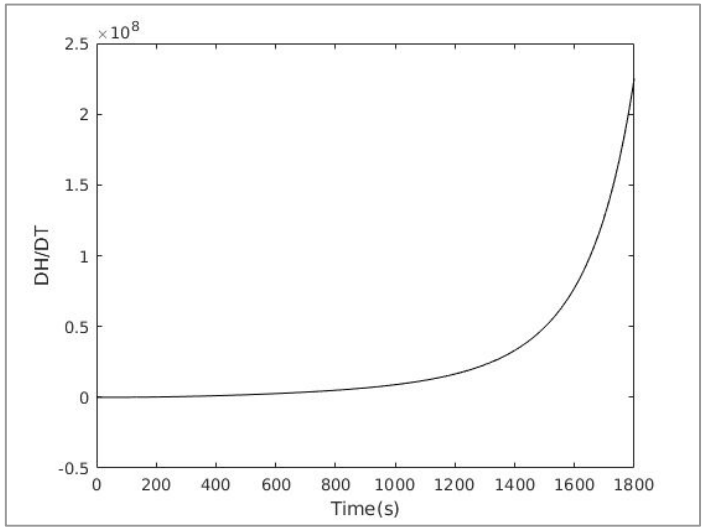


Iteration 1

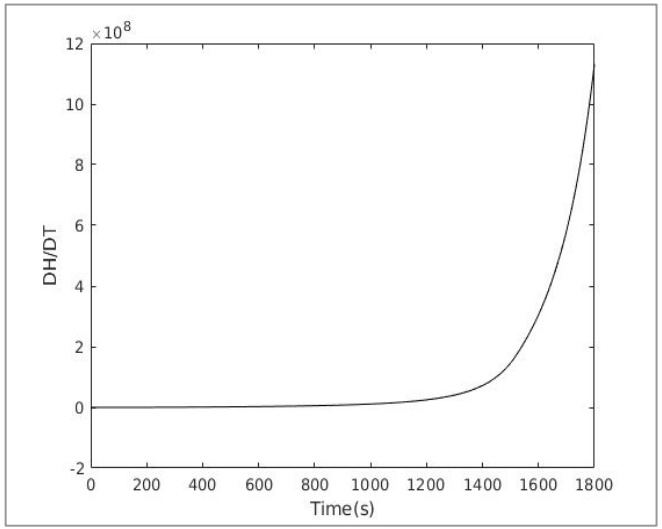


Iteration 2

Results

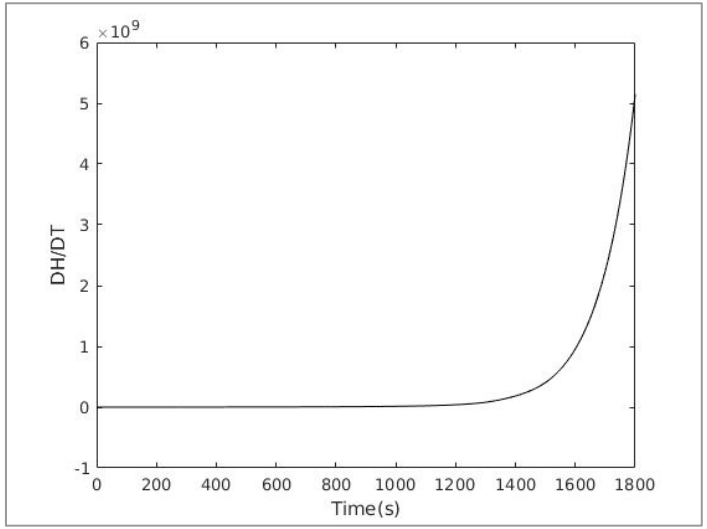


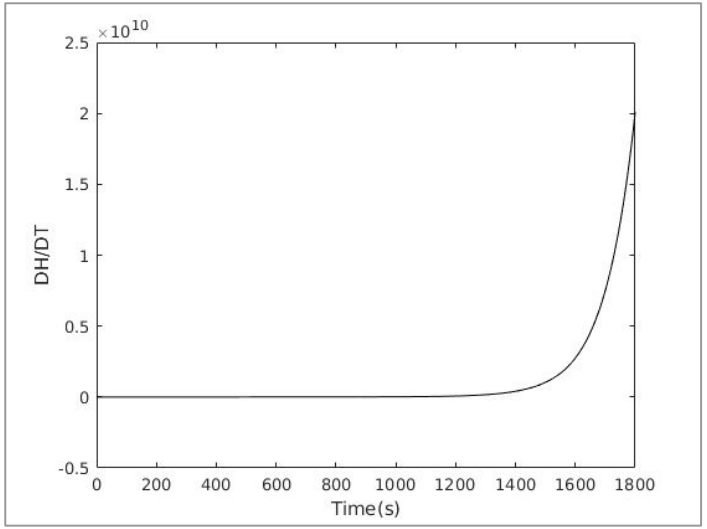
Iteration 3



Iteration 4

Results





Iteration 5

Iteration 6

Uncertainty Quantification

The Need for Uncertainty Quantification

- The kinetic parameters are generally empirical constants determined by fitting experimental data to the model, and, hence, are a source of uncertainty within the system

kinetic constants	value from experiments/ model fitting	range of values
	Uncertainty G	
k_g	1.44×10^8 μm s^{-1}	1.368×10^8–1.512×10^8
E_g/R	4859 K	4616.05–5101.95
g	1.5	1.425–1.575
	Uncertainty B	
k_b	285 $(s\ \mu m^3)^{-1}$	270.75–299.25
E_b/R	7517 K	7141.15–7892.85
b	1.45	1.3775–1.5225

$$B(t) = k_b \exp\left(\frac{-E_b}{RT}\right)\left(\frac{C - C_s(T)}{C_s(T)}\right)^b \mu_3(t)$$

$$G(t) = k_g \exp\left(\frac{-E_g}{RT}\right)\left(\frac{C - C_s(T)}{C_s(T)}\right)^g$$

Stochastic Optimal Control of a Batch Crystallizer

- The time-dependent uncertainties are incorporated into the model equations through stochastic processes known as **Ito processes**.

$$dy = a(y, t)\,dt + b(y, t)\,dz$$

- **dz** is the increment of the Wiener process(Brownian Motion) equal to $\boldsymbol{\varepsilon_t(\Delta t)^{1/2}}$, and **a(y,t)** and **b(y,t)** are known functions. The random value ε_t has a unit normal distribution with zero mean and a standard deviation of 1.
- The equations for state variables get updated to stochastic differential equations.
- For example :

$$\frac{dy_1}{dt} = -3\rho k_v G(t)(y_4 + y_8)$$

$$dY_i = f(\overline{Y}_i, t)\Delta t + g_i \varepsilon_i \sqrt{\Delta t}$$

$$dy_1 = [-3\rho k_v G(t)(y_4 + y_8)]\Delta t + g_1 \varepsilon_1 \sqrt{\Delta t}$$

Problem Definition

- Objective function :

$$\max_{T} L = \mathbf{E}\left[\mu_3^s(t_f) - \mu_3^n(t_f)\right]$$

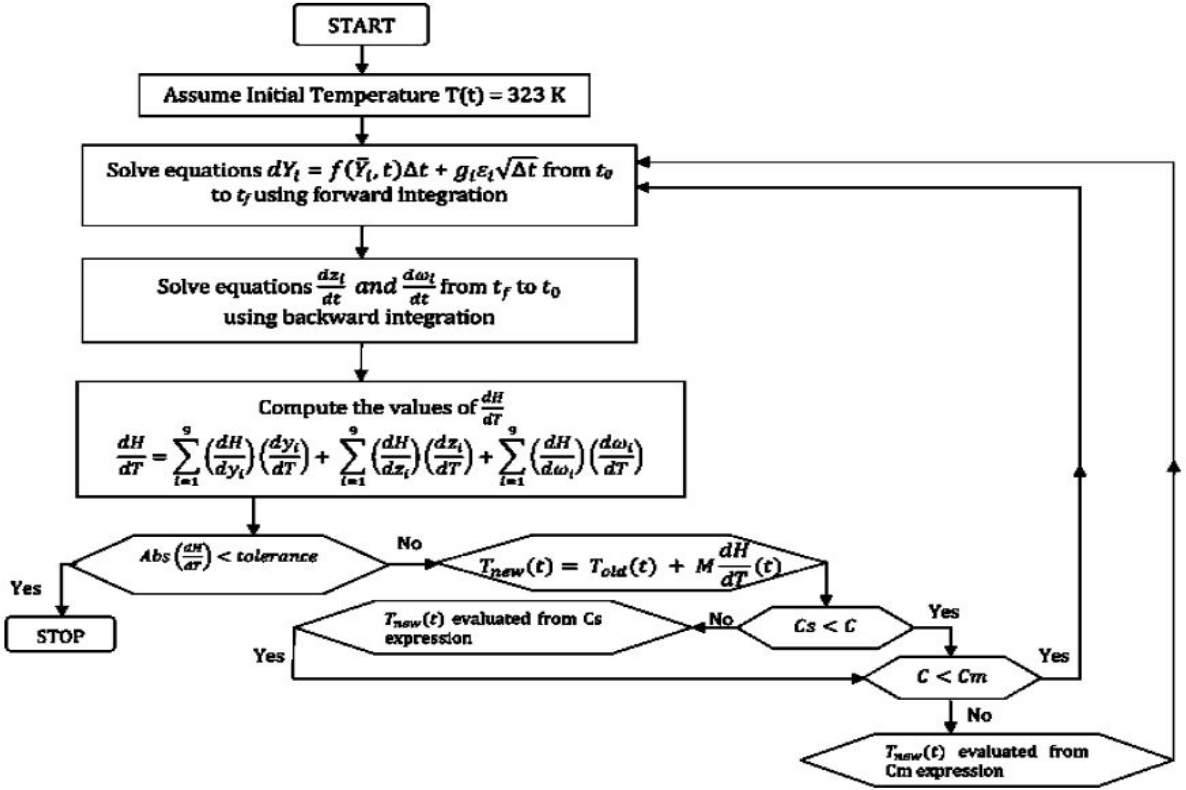
- Active Constraints :

$$C_s \leq C \leq C_m$$

- The optimization problem is solved similarly as the Deterministic Case. The difference lies in the integration of Stochastic Differential Equations using **SDE-Toolbox** in **Matlab.**

$$T^{new}(t) = T^{old}(t) + M\left(\frac{dH}{dT}\right)$$

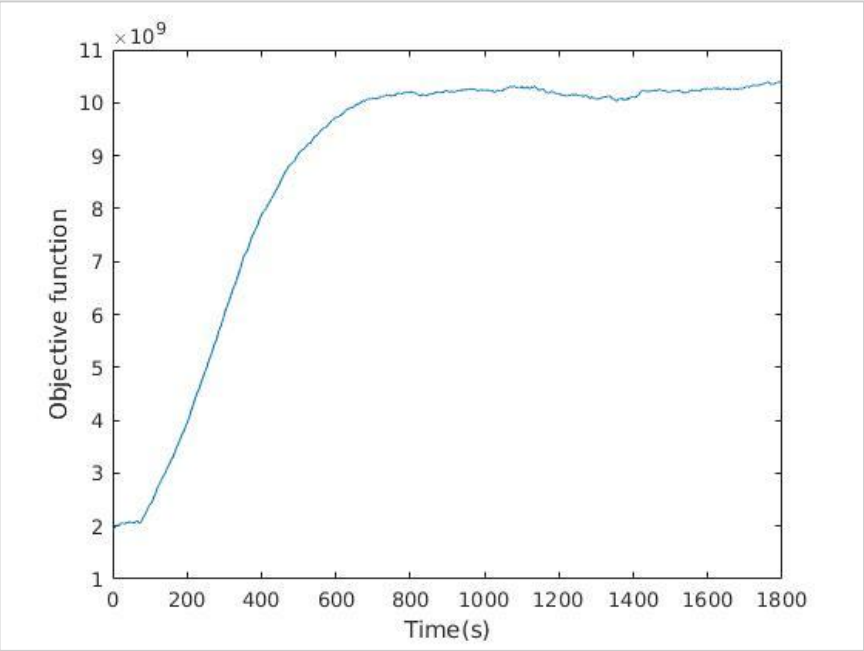
Algorithm



Overall Flowchart

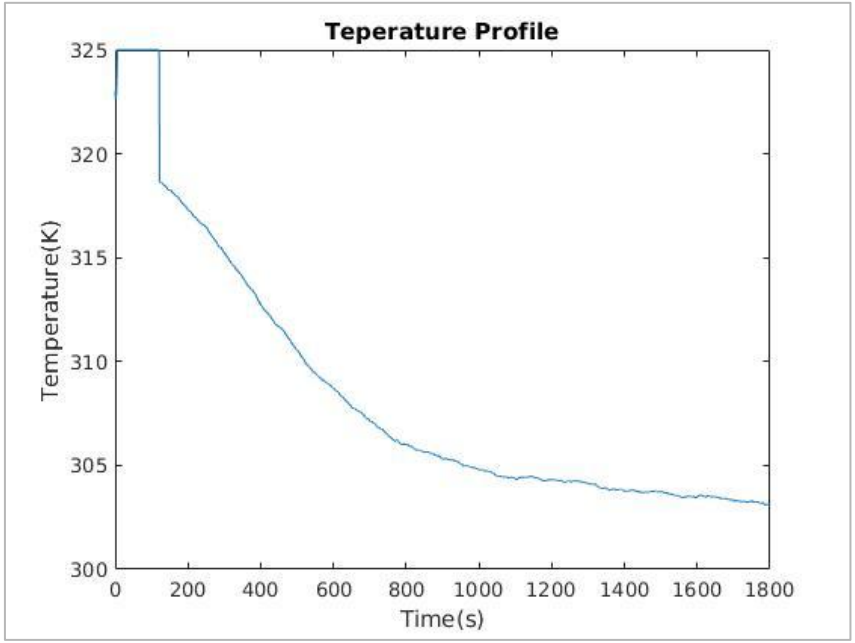
Image Source : Yenkie et al.

Results



- It reaches a maximum value of 9.978 * 10^9 at t = 1800 s which is higher than the deterministic case
- The optimum values are unstable and varies with small amplitude.
- The implementation has been done in **Matlab.**

Results



- The temperature profile decreases abruptly.
- It goes down to reach a value of around 303 K.
- Same fluctuations can be seen at the end of the time horizon.

Polynomial Chaos Expansions(P.C.E)

- A Polynomial Chaos Expansion describes a random process as a spectral expansion of random variables(θi), using orthogonal basis functions, Φi

$$y^d = a_0^d \Phi_0 + \sum_{i_1=1}^{\infty} a_{i1}^d \Phi_1(\theta_{i_1}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} a_{i_1 i_2}^d \Phi_2(\theta_{i_1}, \theta_{i_2}) + \sum_{i_1=1}^{\infty} \sum_{i_2=1}^{i_1} \sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}^d \Phi_3(\theta_{i_1}, \theta_{i_2}, \theta_{i_3})$$

- It is approximated as :

$$y^d \approx \sum_{i=1}^{P_{PCE}} a_i^d \Phi_i(\theta)$$

- It uses a polynomial approximation to introduce the variance in the parameters and is found to be more efficient than traditional methods for solving complex nonlinear systems.

Problem Definition

- Given a process model with uncertain output,

$$y_i = f(x(\theta), \lambda_i(\theta))$$

  where, x is the uncertain input and λ is the uncertain parameter,

- **Aim** is to quantify uncertainty in y(θ) from x(θ) and λ(θ) using the process model.
- The first step is to construct PCEs of x(θ), and λ(θ) using the expressions :

$$x(\theta) = \sum_{i=1}^{P_{PCE}} x_i \phi(\theta) \qquad \lambda(\theta) = \sum_{i=1}^{P_{PCE}} \lambda_i \phi(\theta)$$

$$x_i = \frac{\int x \phi_i(\theta) g(\theta) d\theta}{\langle \phi_i^2 \rangle} \qquad \lambda_i = \frac{\int \lambda \phi_i(\theta) g(\theta) d\theta}{\langle \phi_i^2 \rangle}$$

Usage of PCE in Batch Crystallization

- The batch crystallizer consists of 9 state variables given by :

$$y_i = [C \quad \mu_0^s \quad \mu_1^s \quad \mu_2^s \quad \mu_3^s \quad \mu_0^n \quad \mu_1^n \quad \mu_2^n \quad \mu_3^n]$$

- The outputs of the model become uncertain due to the existence of variation in 6 kinetic parameters λi = kg, g, Eg, kb, b and Eb.

- This work follows a **Non-Intrusive approach** which involves evaluating the model at N sample points to approximate the deterministic coefficients.

- The samples are drawn by constructing a joint distribution of the kinetic parameters.

- For each of the above sample, the optimization problem is solved using the Steepest Ascent Hamiltonian method

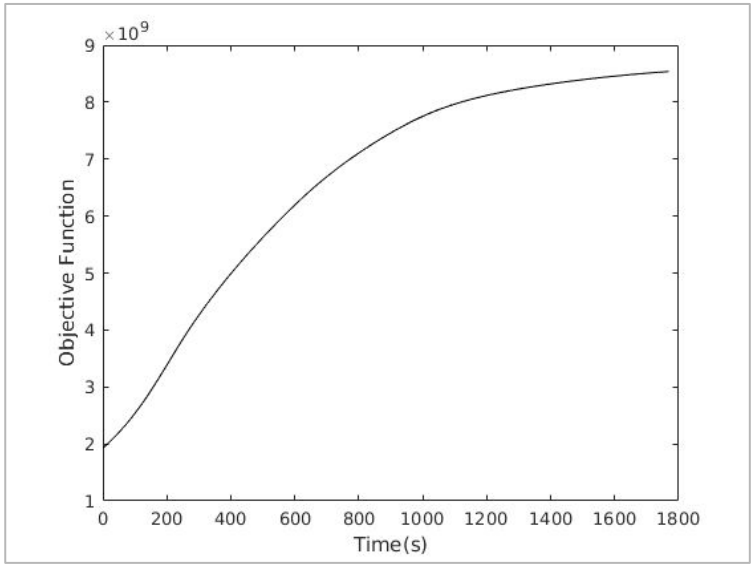
$$y_i = \frac{1}{\langle \phi_i^2 \rangle} \frac{1}{N} \sum_{j=1}^{N} y^j \phi_i(\theta)$$

Results

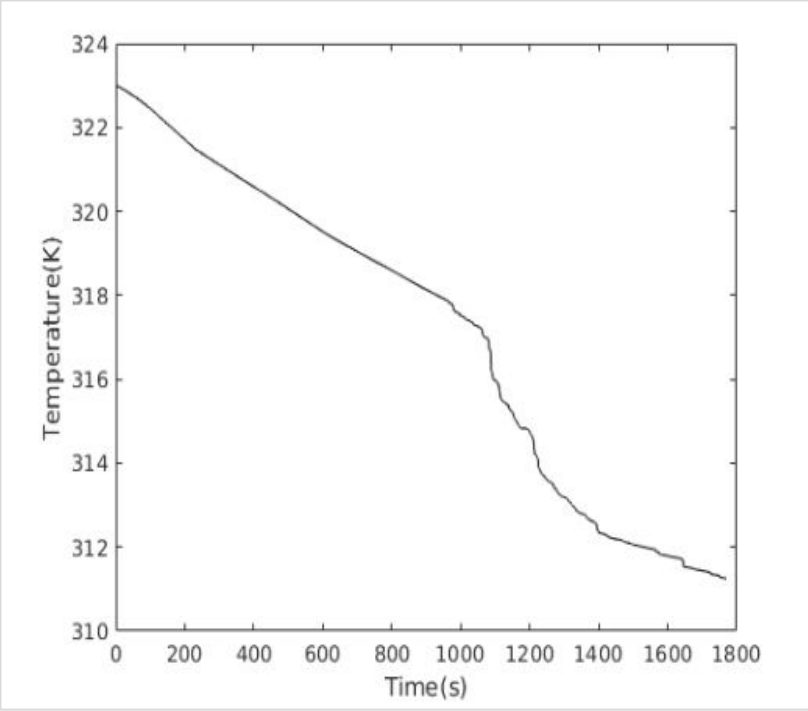
- As the above Equation averages over N samples, the resultant maximises the objective function :

$$\max_{T} L = \mathbf{E}\left[\mu_3^s(t_f) - \mu_3^n(t_f)\right]$$

- The following profile was obtained :



Results



- The implementation was performed in **Python** by using **chaospy** library for generating samples and determining coefficients.
- A python source code was used for evaluating optimum Temperature profile for each sample.
- The cooling carries on to about 311 K.

Application to Unseeded Crystallization

Case Study

- To build a predictive model for unseeded batch crystallization of **L-Asparagine Monohydrate(LAM)** crystals using kinetics developed at our lab.
- Population Balance Equations also hold valid for these crystals.
- The key differences :

$$B = k_{j_1} S \exp\left(-k_{j_2} \frac{\ln^3 C_c/C^*}{\ln^2 S}\right) \qquad G = k_g (S-1)^g$$

- The new process parameters get reduced to 4 : Kj1, Kj2, Kg and g

Problem Definition

- The model developed in this work has been extended to LAM crystals to prove the validity of **PCE** with the **Hamiltonian Optimization Scheme**.

- Objective Function now involves maximising the weight mean size of the crystals by optimising the temperature profile :

$$\max_{T(t)} \phi = \mu_4/\mu_3 \quad at \quad t_f$$

- No seeding has been done, therefore **state variables** are now defined as :

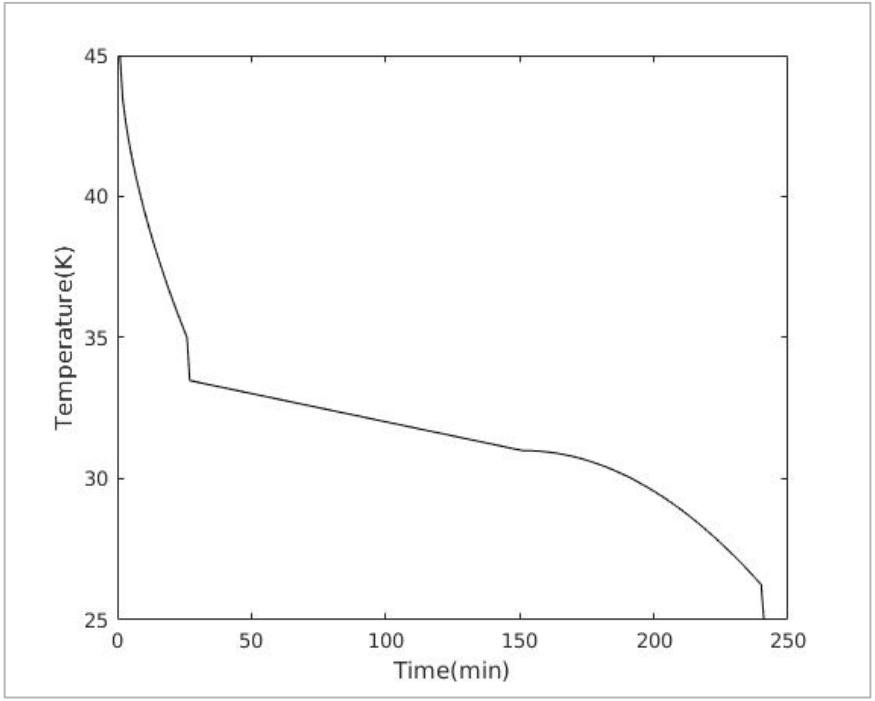
$$y_i = [\quad C \quad \mu_0 \quad \mu_1 \quad \mu_2 \quad \mu_3 \quad \mu_4 \quad]$$

- **State Equations** :

$$\frac{du_0}{dt} = B$$

$$\frac{du_j}{dt} = jG\mu_{j-1}$$

Results



- The temperature profile obtained here confirms with the one obtained in the original work.
- It consists of 3 regions of cooling corresponding to crystallization of LAM crystals.
- The maximised value of the objective function was obtained at : 300μm

Conclusions

- An analysis of 3 different methods of Optimal Control was done for a batch cooled crystallization process which produced effective results.

- After comparing the final values of the objective functions[particle volume] the following values were obtained :
  1. Deterministic : **9.153 × 10^9 µm^3**
  2. Expected value for Stochastic involving Ito Processes : **9.978 × 10^9 µm^3**
  3. Expected value for Stochastic case involving PCE : **8.64 × 10^9 µm^3**

- The validity of the novel approach of PCE was reaffirmed when applied to an existing crystallization problem.

- The model maximises the value of objective function at **300µm** which is at par with other cooling policies such as cubic cooling policy(251µm).

- This proves the efficacy of P.C.E in the field of batch crystallization

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Thank You