CHAPTER 3

THEORY

This chapter defines the theory that involves this research. It consists of three subjects as follows.

3.1 Rinsing Process

3.1.1 Rinsing Principle

B. Kusher and S. Kusher [1994] explained a principle of water rinsing which is a dilution process involved mass transfer principle. Mass which trap on the surface of workpiece or the barrel of workpiece is transferred to water in rinsing tank. A mechanism of mass transfer consists of diffusion and convection.

Diffusion is atomic process. Atom or molecule of matter that dissolves in water moves to other atom such as water. Mass transfer of this mechanism occurs from a difference between concentration of the solution at surface of workpiece with high value and concentration of the solution in rinsing tank with small value. Diffusion depends on each characteristic of molecular movement and slowly occurs. The velocity of diffusion depends on the temperature and size of diffusion molecule comparison size of molecule.

Convection is a movement of matter in liquid layer. Matter that dissolves in water moves to liquid layer such as water. This mechanism can put the external power such as mixing, pumping and vibrating to accurate fast mass transfer.

The rinsing process can be explained with a simple model with called "Tank-in-Tank Rinsing Model". Based on assumption, workpiece or barrel which is rinsed has one tank with a trapped chemical and dipping in rinsing tank. The effective mixing rate, k related on making material balance.

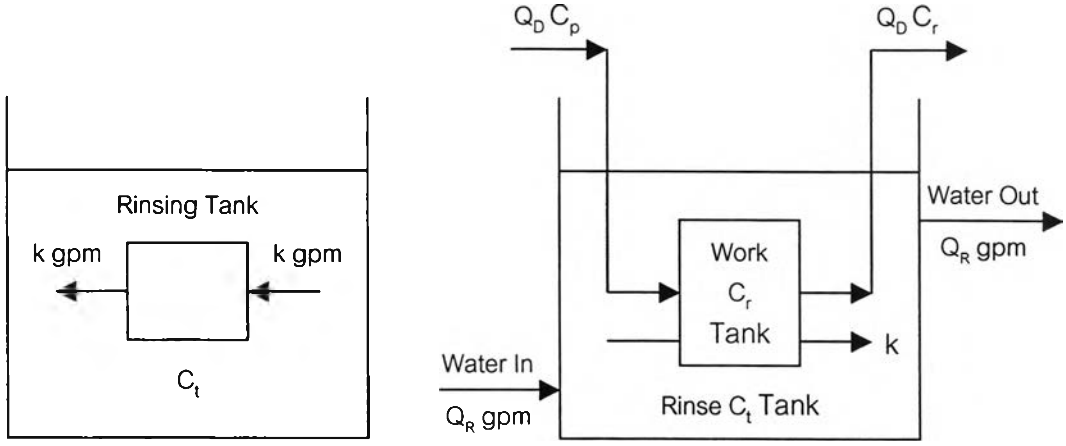

Figure 3.1 Tank-in-Tank Rinsing Model for drag out and rinse overflow rinsing

From figure 3.1, the model can be formulated for a material balancing equation in a differential form and a material balancing equation at steady state following.

Drag Out Rinse

At workpiece or barrel
$$dC_r = \left(\frac{k}{Q_D}\right)(C_t - C_r)dt \qquad (3.1)$$

At rinsing tank
$$dC_t = \left(\frac{k}{V}\right)(C_r - C_t)dt \qquad (3.2)$$

At steady state, solving the equation 3.1 and 3.2, we get

At workpiece or barrel
$$C_r = \left(\frac{Q_D C_p}{V}\right)\left[1 + \left(\frac{V}{D}\right)\exp\left(\frac{-kt}{Q_D}\right)\right] \qquad (3.3)$$

At rinsing tank
$$C_t = \left(\frac{Q_D C_p}{V}\right)\left[1 - \exp\left(\frac{-kt}{Q_D}\right)\right] \qquad (3.4)$$

Rinse Overflow Rinsing

At workpiece or barrel $$dC_r = (C_p + k\frac{C_t}{Q_D} - C_r - k\frac{C_r}{Q_D})dt \quad (3.5)$$

At rinsing tank $$dC_t = (k\frac{C_r}{V} - k\frac{C_t}{V} - Q_R\frac{C_t}{V})dt \quad (3.6)$$

At steady state, solving the equation 3.5 and 3.6, we get

At workpiece or barrel $$C_r = \frac{C_p}{(1+\frac{Q_R}{Q_D}+\frac{Q_R}{k})} \quad (3.5)$$

At rinsing tank $$C_t = \frac{C_p}{(1+\frac{Q_R}{Q_D}+\frac{Q_R}{k})} \quad (3.6)$$

Above equations, if a rinsing process has a high the effective mixing rate ($k=\infty$), the mechanism of this process is similar with perfect mixing assumption.

3.1.2 Type of Rinsing Process

Now, the rinsing process has several types, which depend on the objective and area of factory. Type of rinsing process can be divided as follows.

1) Drag Out Rinse

Drag out rinse is rinsing of work piece by immersing it in a rinsing tank with no fresh rinse of water feed. Therefore, concentration of chemical in the tank is increase when rinsing time raise. Sometime, rinse water in the tank is discharged or recycled for chemical preparation, when the concentration rises to a limitation.

For a continuous operation, the equation of drag-out rinse at steady state is expressed as (3.7).

$$C = C_p\left[1-\exp(\frac{Q_o}{V})\right] \quad (3.7)$$

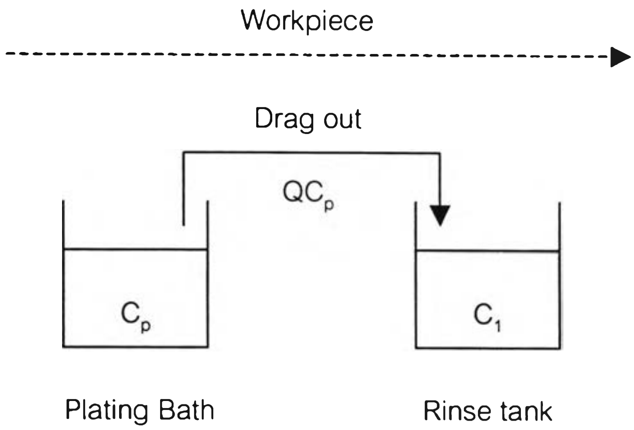

Figure 3.2 Drag out rinse

2) Overflow Rinsing

The rinse tank has continuous flow of fresh rinse water. The water overflows from rinse tank is wastewater.

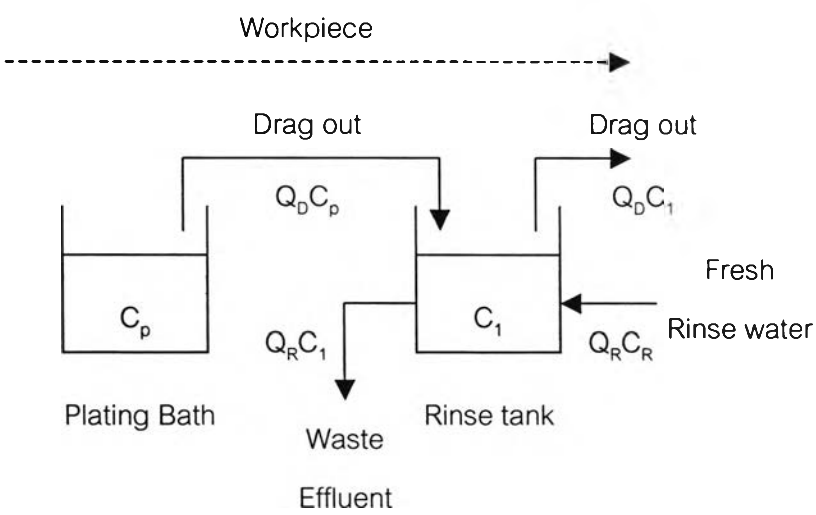

Figure 3.3 Overflow rinse

At steady state and complete mixing, the equation for overflow rinse is given by (3.8).

$$C = Q_D\left[\frac{C_P}{Q_D + Q_R}\right] \quad (3.8)$$

If the flow rate of rinse water is very large with volume of drag out $(Q_R > 10Q_D)$, term of $(Q_D + Q_R)$ can be reduced to Q_R as (3.9).

$$C = Q_D\left[\frac{C_P}{1 + A}\right] \quad (3.9)$$

Where $A = \frac{Q_R}{Q_D}$

3) **Cascade Rinsing**

These type has continuous flow of fresh rinse water too, but saving of rinse water usage is higher than overflow rinse. Cascade rinsing type has more two rinse tanks with overflow water from the last tank flows to the first tank and the overflow water from the first tank discharge to wastewater treatment plant. Normally, cascade rinsing which is widely used classifies two types as follows.

Series Type

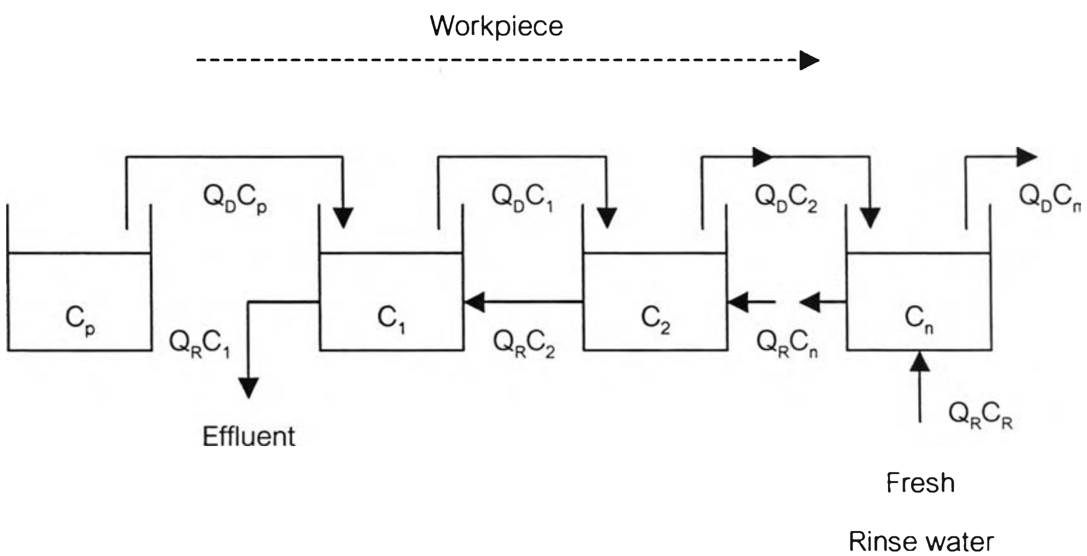

Figure 3.4 Series type of cascade rinsing

Parallel Type

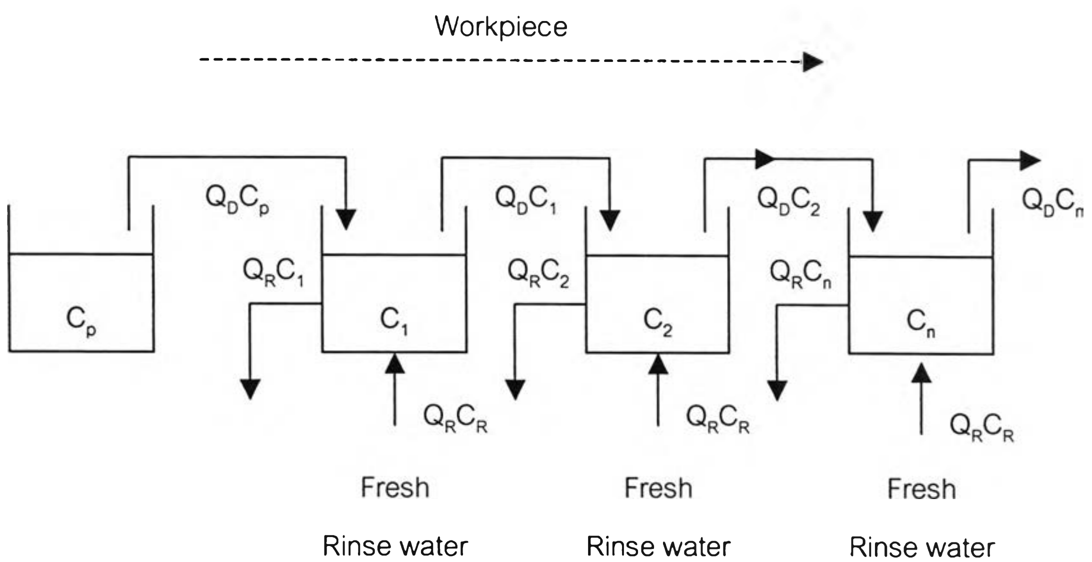

Figure 3.5 Parallel type of cascade rinsing

At steady state and complete mixing, the equation of series and parallel types of cascade rinsing are given by (3.10 and 3.11).

Series type $$C_n = C_p\left[\frac{A-1}{A^{n+1}-1}\right] \tag{3.10}$$

Parallel type $$C_n = C_p(1+A^n) \tag{3.11}$$

Where n = number of rinse tank

The words often use for the overflow rinsing type such as rinse ratio, dilution ratio, or rinse criteria. It has a same meaning, which means a ratio of requirement volume of rinse water consumption for rinsing workpiece. These volumes can be calculated from

$$\frac{C_p}{C} = \left(\frac{Q_R}{Q_D}\right)^n \tag{3.12}$$

All equation (3.7 to 3.12) with a simple form at steady state frequently uses to calculate an optimum volume of water consumption for high rinsing efficiency. It means concentration of contaminant at final state that isn't over an acceptable criterion.

3.2 Modeling of Rinsing Process

Zofia Buczko [1992] presented a mathematical model about rinsing process. He required to estimate the contaminants on the workpiece surface after rinsing. The complete-mixing theory is the simplest but is far from practices. However, it is still the basic assumption made in all rinsing equation. Some attempts at analysis of the concentration on the workpiece after rinsing have been made. They were mainly based on diffusion and convection theories. The mathematical expressions derived were related to ideal conditions, which cannot exist in a real system.

When analysis the results of the laboratory investigations, it has been concluded that when modeling the rinsing process mathematically it is not possible to apply diffusion or convection equations. The hydrodynamics of these processes is much more complicated to express by simple physical theory.

Because of contrary to the assumption of complete equalization of concentration at the product and in a rinsing tank during the washing process, he assumed that an average concentration C_n at the workpiece after rinsing in the n th rinse tank is a combination of the concentration C_{n-1} of the inlet solution (concentration at the workpiece after rinsing in the n-1 th rinse tank) and an average final concentration Z_n the tank taken in suitable proportions. The average concentration of the workpieces can be described by

$$C_n = a_n C_{n-1} + (1 - a_n) Z_n \tag{3.13}$$

The coefficient a_n indicates the contribution from the initial concentration to the average final concentration at a workpiece after rinsing. It is called the imperfect-mixing coefficients (IMCs) with values from 0 to 1. The IMCs are a_n=0 in the case of perfect mixing. It also depends on the rinsing techniques and character of the withdrawn film on the work surface.

To formulate the rinsing equation, an additonal assumption of continuous-rinsing operation has also been made. In fact the rinsing process in a given rinse is not continuous but stepwise; workpieces are immersed within pre-determined time intervals. If the volume of drag-out solution is small with respect to the rinse volume, the concentration variations in the rinses can be treated as pseudo-continuous with time and differential calculus can be applied for calculation. Under this assumption the computational mass balance equations have been derived previously and are usually used in perfect-mixing rinsing calculations.

A differential equation for the n th non-flow rinse is derived, under the assumption that for each rinse the drag-out D is the same bath before and after rinsing:

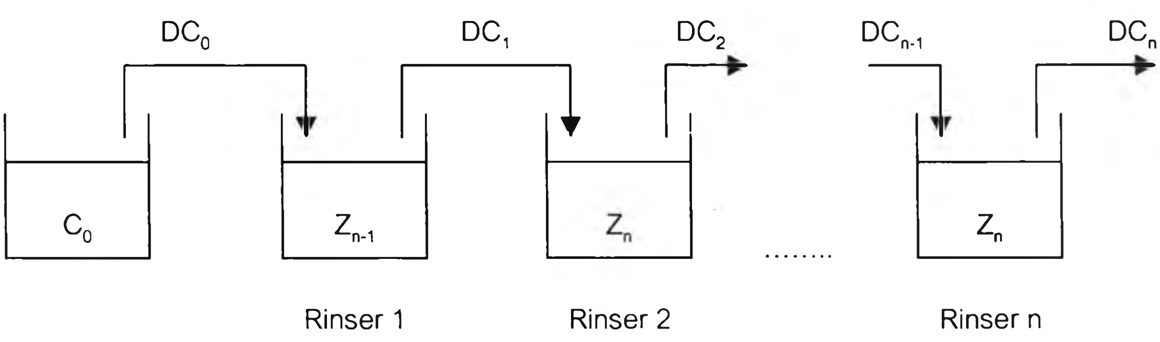

Figure 3.6 Rinsing system

$$DC_{n-1} = V\frac{dZ_n}{dt} + DC_n \qquad n = 1,2,3,... \tag{3.14}$$

with the initial condition Z_n (t=0) =0, where V is the volume of the rinsing bath and C_0 is the concentration fo the process of bath drag into the first rinse, which is invariant in time.

For incomplete mixing, substitution of equation (3.13) into (3.14) and rearrangement one can obtain the following set of differential equations

$$\left.\begin{aligned} kb_nC_{n-1} &= \frac{dZ_n}{dt} + kb_nC_n \\ C_n &= aC_{n-1} + (1-a_n)Z_n \end{aligned}\right\} n = 1,2,3,... \tag{3.15}$$

Where $b_n = 1 - a_n, k = \frac{D}{V}$

One can find that the solution is of the form

$$\left.\begin{aligned} C_n &= C_0\left(1 - \sum_{j=1}^{n} \alpha_n^j \exp(-kb_jt)\right) \\ Z_n &= C_0\left(1 - \sum_{j=1}^{n} \beta_n^j \exp(-kb_jt)\right) \end{aligned}\right\} n = 1,2,3,... \tag{3.16}$$

Where the recurrent form for the coefficienta α_n^j and β_n^j is

$$\left.\begin{aligned} \beta_n^j &= 1 \\ \alpha_n^j &= b_1 \end{aligned}\right\} \text{for } n = 1, j = 1$$

$$\left.\begin{aligned} \beta_n^j &= \frac{b_n}{b_n - b_j}\alpha_{n-1}^j \\ \alpha_n^j &= \alpha_n \alpha_{n-1}^j + b_n \beta_n^j \end{aligned}\right\} \text{for } n > 1, j = 1,\ldots,n\text{-}1 \tag{3.17}$$

$$\left.\begin{aligned} \beta_n^n &= 1 - \sum_{i=1}^{n-1} \frac{b_n}{b_n - b_j}\alpha_{n-1}^j \\ \alpha_n^n &= b_n \beta_n^n \end{aligned}\right\} \text{for } j = n$$

In case perfect mixing (a=0 and b=1), it is easy to obtain an equation.

$$C_n = C_0\left(1 - \exp(-kt)\sum_{j=0}^{n-1}\frac{(kt)^j}{j!}\right) \tag{3.18}$$

Based on equation 3.16, 3.17 and 3.18, the dynamics behavior of concentration in each rinse stage is shown in figure 3.7 and 3.8 following.

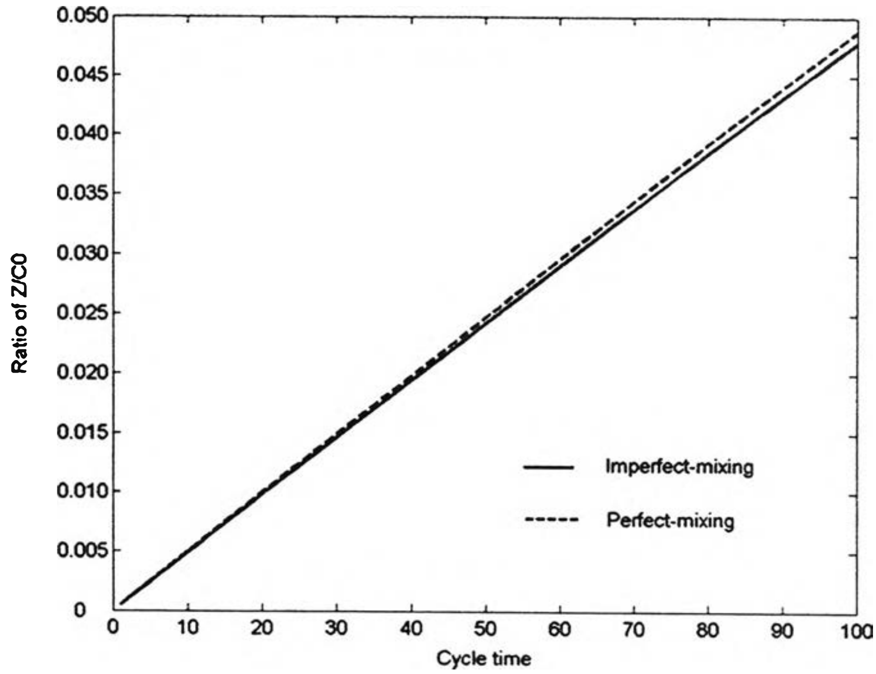

Figure 3.7 Dynamics response of concentration in the first rinse stage

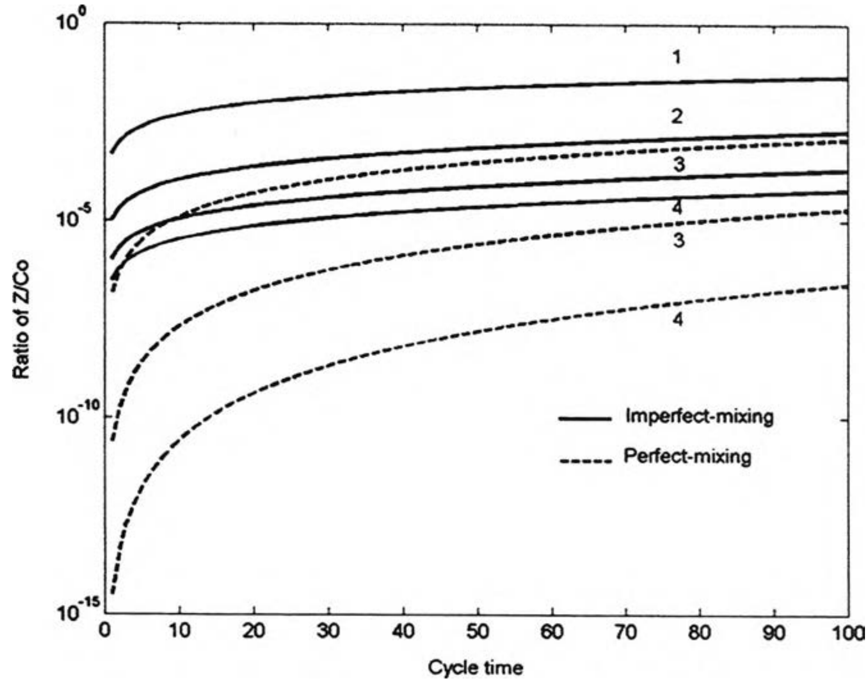

Figure 3.8 Dynamics response of concentration in four rinse stages

3.3 Optimization

Optimization is a method to obtain the best solution under constraint of system or process. The odjective function is identified the best solution. It is determined from asset, operation cost, production, net profit and other. The value of the objective function can be found by adjust decision variable of system. This variable maybe is size of equipment and operating condition of process such as pressure, temperature and flowrate etc. Adjusting this variable must consider under constraint of operation as purity of product, fesibility of model and the relationship of variable.

The optimization consist of four parts as following.

Process Model

The objective of model is to identify the solution of objective function and the position of constraint. A reliable model is necessary for calculation which can be devided as mathematical model and actual process

Objective Function

The objective function means a equation or group of equation which are formulated for calculation. The caculation have finding minimum value or finding maximum value. The objective function for optimization has various form such as annual cost, net benefit, production time and energy consumption rate etc.

Constraint

The optimization always has contraint of eah system for finding the solution in feasible region of decision variable. The feasible region of decision varible is determine with constraint which is formulated from mass balance, energy balance, equipment design and property of matter.

Natural condition of physical production is express area or feasible region and the solution locates in this region. The constraint has two forms as following.

- Equality constraint is a constraint which has a sign (=) in the equation. The equality constraint is an equation which indicates process and product limitation such as mass balance, energy balance and purity of product.

- Inequality constraint is a constraint which has sign (=), (<) ,(>), ($\leq$), ($\geq$) or ($\neq$) in the equation The inequality constraint is an equation which indicates limitation of design and other limitation such as mole fraction, no negative value of flowrate and minimum of production rate.

Decision Variable

Decision variable is adjust variable for finding maximum or minimum of objective function value and affecting objective function such as temperature, pressure, flowrate, concentration and reactor size. In the practicality, decision varible is set point for process control system.

The optimization problem can be classified two categories as follows

1. Static optimization is the process of minimizing or maximizing the cost or benefits of some objective function for one instant in time only.

2. Dynamic optimization is the process of minimizing or maximizing the cost or benefits of objective function over a period of time.

Characterisitc of dynamics optimization problems can be divied that

3.3.1 Free Dynamic Optimization

Discrete Time

We focus on the problem of controlling the system

$$x_{i+1} = f(x_i, u_i) \qquad i = 0,\ldots,N\text{-}1 \qquad x_0 = \underline{x}_0 \qquad (3.19)$$

such that the cost function

$$J = \phi(x_N) + \sum_{i=0}^{N-1} L(x_i, u_i) \tag{3.20}$$

is minimized. The solution to this problem is a sequence of control actions or decisions, $u_i = 0,...N-1$. Knowing the sequence $u_i = 0,...N-1$, the solution is the path or trajectory of the state and the costate. The problem is specified by the functions f, L and ϕ, the horizon N and the initial state $\underline{x}_0$.

The problem is an optimization of (3.20) with $N+1$ set of equality constraints given in (3.19). Each set consists of n equality constraints. We associated a vector, λ of Lagrange multipliers to each set of equality constraints. By tradition λ_{n+1} is associated to $x_{i+1} = f(x_i, u_i)$. These vectors of Lagrange multipliers often denoted as costate or adjoint state.

The Hamiltonian function with is a scalar function is defined as

$$H_i(x_i, u_i, \lambda_{i+1}) = L_i(x_i, u_i) + \lambda_{i+1}^T f_i(x_i, u_i) \tag{3.21}$$

and facilitates a very compact formulation of the necessary conditions for an optimum.

Considering the free dynamic optimization problem of the system (3.19) from the initial state, the performance index (3.20) is minimized. The necessary condition is given by the Euler-Lagrange equations (for $i = 0,...,N-1$):

$$x_{i+1} = f(x_i, u_i) \quad \text{State equation} \tag{3.22}$$

$$\lambda_i^T = \frac{\partial}{\partial x_i} H_i \quad \text{Costate equation} \tag{3.23}$$

$$0^T = \frac{\partial}{\partial u_i} H_i \quad \text{Stationarity condition} \tag{3.24}$$

and the boundary conditions

$$x_0 = \underline{x}_0 \qquad \lambda_N^T = \frac{\partial}{\partial x}\phi(x_N) \tag{3.25}$$

which is a split boundary condition.

The necessary condition can also be expressed in a more condensed form as

$$x_{i+1}^T = \frac{\partial}{\partial \lambda}H_i \qquad \lambda_i^T = \frac{\partial}{\partial x}H_i \qquad 0^T = \frac{\partial}{\partial u}H_i \tag{3.26}$$

with the boundary conditions:

$$x_0 = \underline{x}_0 \qquad \lambda_N^T = \frac{\partial}{\partial x}\phi(x_N) \tag{3.27}$$

The Euler-Lagrange equations express the necessary conditions for optimality. The state equation (3.22) is inherently forward in time, whereas the costate equation, (3.23) is backward in time. The stationarity condition (3.24) links together the two set of recursions as indicated in figure 3.9.

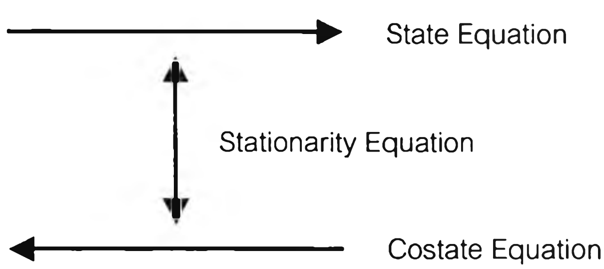

Figure 3.9 Charateristics of Euler – Lagrange equation for discrete time free dynamics optimization

The state equation (3.22) is forward in time, whereas the costate equation, (3.23), is backward in time. The stationarity condition (3.24) links together the two set of recursions.

Continuous Time

Consider the problem related to finding the input function U_t to the system

$$\dot{x} = f_t(x_t, u_t) \qquad x_0 = \underline{x}_0 \qquad t \in [0, T] \tag{3.28}$$

such that the cost function

$$J = \phi_T(x_T) + \int_0^T L_t(x_t, u_t)dt \tag{3.29}$$

is minimized. Here the initial state $\underline{x}_0$ and final time T are given (fixed). The problem is specified by the dynamic function, f_t, the scalar value functions ϕ and L and the constants T and $\underline{x}_0$.

The problem is an optimization of (3.29) with continuous equality constraints. Similarilly to the situation in discrete time, we here associate a n-dimensional function, λ_t, to the equality constraints, $\dot{x} - f_t(x_t, u_t)$. Also in continuous time these multipliers are denoted as costate or adjoint state. In some part of the litterature the vector function, λ_t, is denoted as influence function.

For convienence we can introduce the scalar Hamiltonian function as follows:

$$H_t(x_t, u_t, \lambda_t) = L_t(x_t, u_t) + \lambda_t^T f_t(x_t, u_t) \tag{3.30}$$

We are now able to give the necessary condition for the solution to the problem.

Consider the free dynamic optimization problem in continuous time of bringing the system (3.28) from the initial state such that the performance index (3.29) is minimized. The necessary condition is given by the Euler-Lagrange equations (for $t \in [0, T]$):

$$\dot{x}_t = f_t(x_t, u_t)$$ State equation (3.31)

$$-\dot{\lambda}_t^T = \frac{\partial}{\partial x_t} H_t$$ Costate equation (3.32)

$$0^T = \frac{\partial}{\partial u_t} H_t$$ Stationarity condition (3.33)

and the boundary conditions

$$x_0 = \underline{x}_0 \qquad \lambda_T = \frac{\partial}{\partial x}\phi_T(x_T) \tag{3.34}$$

We can express the necessary conditions as

$$\dot{x}^T = \frac{\partial}{\partial \lambda} H \qquad \dot{\lambda}^T = \frac{\partial}{\partial x} H \qquad 0^T = \frac{\partial}{\partial u} H \tag{3.35}$$

with the (split) boundary conditions

$$x_0 = \underline{x}_0 \qquad \lambda_T = \frac{\partial}{\partial x}\phi_T \tag{3.36}$$

3.3.2 Dynamic Optimization with End Points Constraints

Consider the discrete time system (for $i = 0,1,\ldots,N-1$)

$$x_{i+1} = f(x_i, u_i) \qquad x_0 = \underline{x}_0 \tag{3.37}$$

the cost function

$$J = \phi(x_N) + \sum_{i=0}^{N-1} L(x_i, u_i) \tag{3.38}$$

and the simple terminal constraints

$$x_N = \underline{x}_N \tag{3.39}$$

where $\underline{x}_N$ and $\underline{x}_0$ are given. In this simple case, the terminal contribution, ϕ, to the performance index could be omitted, since it has not effect on the solution (except a constant additive term to the performance index). The problem consists of the system (3.37) from its initial state $\underline{x}_0$ to a (fixed) terminal state $\underline{x}_N$ such that the performance index, (3.38) is minimized.

The problem is specified by the functions f and L (and ϕ), the length of the horizon N and by the initial and terminal state $\underline{x}_0$, $\underline{x}_N$. We apply the usual notation and associate a vector of Lagrange multipliers λ_{n+1} to each of the equality constraints $x_{i+1} = f(x_i, u_i)$. To the terminal constraint we associate, υ which is a vector containing n (scalar) Lagrange multipliers.

As in the unconstrained case, we introduce the Hamiltonian function

$$H_i(x_i, u_i, \lambda_{i+1}) = L_i(x_i, u_i) + \lambda_{i+1}^T f_i(x_i, u_i) \tag{3.40}$$

and obtain a much more compact form for necessary conditions, which is stated in the theorem below.

Considering the dynamic optimization problem of the system (3.37) from the initial state, $\underline{x}_0$, to the terminal state, $\underline{x}_N$, the performance index (3.38) is minimized. The necessary condition is given by the Euler-Lagrange equations (for $i = 0,\dots,N-1$)

$$x_{i+1} = f(x_i, u_i) \qquad \text{State equation} \tag{3.41}$$

$$\lambda_i^T = \frac{\partial}{\partial x_i} H_i \qquad \text{Costate equation} \tag{3.42}$$

$$0^T = \frac{\partial}{\partial u_i} H_i \qquad \text{Stationarity condition} \tag{3.43}$$

The boundary conditions are

$$x_0 = \underline{x}_0 \qquad x_N = \underline{x}_N \tag{3.44}$$

and the Lagrange multiplier, υ, related to the simple equality constraints can be determined from

$$\lambda_N^T = \upsilon^T + \frac{\partial}{\partial x_N} \phi \tag{3.45}$$

Notice, the performance index will rarely have a dependence on the terminal state in this situation. In that case

$$\lambda_N^T = \upsilon^T \qquad (3.46)$$

Also notice, the dynamic function can be expressed in terms of the Hamiltonian function as

$$f_i^T(x_i, u_i) = \frac{\partial}{\partial \lambda} H_i \qquad (3.47)$$

and obtain a more memotechnical form

$$x_{i+1}^T = \frac{\partial}{\partial \lambda} H_i \qquad \lambda_i^T = \frac{\partial}{\partial x} H_i \qquad 0^T = \frac{\partial}{\partial u} H_i \qquad (3.48)$$

for the Euler-Lagrange equations, (3.41) - (3.43).

Continuous Time

In this section we consider the continuous case in which $t \in [0,T] \in R$. The problem is to find the input function u_t to the system

$$\dot{x} = f_t(x_t, u_t) \qquad x_0 = \underline{x}_0 \qquad (3.49)$$

such that the cost function

$$J = \phi_T(x_T) + \int_0^T L_t(x_t, u_t)dt \qquad (3.50)$$

is minimized and the end point constraints in

$$\psi_T(x_T) = 0 \qquad (3.51)$$

are met. Here the initial state $\underline{x}_0$ and final time T are given (fixed). The problem is specified by the dynamic function, f_t, the scalar value functions ϕ and L, the end point constraints through the function ψ and the constants T and $\underline{x}_0$.

We can for the sake of convenience introduce the scalar Hamiltonian function as:

$$H_t(x_t,u_t,\lambda_t) = L_t(x_t,u_t) + \lambda_t^T f_t(x_t,u_t) \tag{3.52}$$

As in the previous section on discrete time problems we, in addition to the costate (the dynamics is an equality constraints), introduce a Lagrange multiplier, υ associated with the end point constraints.

Consider the dynamic optimization problem in continuous time of bringing the system (3.49) from the initial state and a terminal state satisfying (3.51) such that the performance index (3.50) is minimized. The necessary condition is given by the Euler-Lagrange equations ($t \in [0,T]$):

$$\dot{x}_t = f_t(x_t,u_t) \qquad \text{State equation} \tag{3.53}$$

$$-\dot{\lambda}_t^T = \frac{\partial}{\partial x_t} H_t \qquad \text{Costate equation} \tag{3.54}$$

$$0^T = \frac{\partial}{\partial u_t} H_t \qquad \text{Stationarity condition} \tag{3.55}$$

and the boundary conditions:

$$x_0 = \underline{x}_0 \qquad \psi_T(x_T) = 0 \qquad \lambda_T = \upsilon^T \frac{\partial}{\partial x}\psi_T + \frac{\partial}{\partial x}\phi_T(x_T) \tag{3.56}$$

which is a split boundary condition.