DSM Updated Equations

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January 2024

1 Introduction

Here we reiterate the equations used for modelling the operation mode switching of Cl_2 production. The equations are corrected wherever necessary and also the missing equations have been provided.

The corrections have been inspired from the paper: Mitra et al, 2013

1.1 Modelling of Transitional Variables

1.1.1 Defining Mode

$$\sum_{(m \in M)} y_{m,t} = 1 \ \forall t \in T$$

1.1.2 Defining Transitions - Correction

Firstly, Defining the variable z:

Since, in the minimum time for each mode constraint, the index of time would till -35 corresponding to the first active mode to be active for at least first 36 time steps,

We define a new set of Time Steps: Just for sake of preventing error while satisfying the constraint (because all the z values below t_1 would anyways be zero only).

$$T_{minassure} = \{-max\{\theta_{mm'}\}, ..., -1, -2, 0, \{T\}\}$$

Also, Note: Initialise the variable value as 0, through all indices.

Fundamental Equations (From Mitra 2013: Opt Schedule)

1.
$$\sum_{(m' \in M)} z_{m'm,t} = y_{m,t} \ \forall m \in M \ \forall t \in T$$

2.
$$\sum_{(m' \in M)} z_{mm',t} = y_{m,t-1} \ \forall m \in M \ \forall t \in T/\{t_1\}$$

When Self-Transition variables are not required, we can write:

$$\sum_{(m' \in M)} z_{m'm,t} - \sum_{(m' \in M)} z_{mm',t} = y_{m,t} - y_{m,t-1} \ \forall m \in M \ \forall t \in T/\{t_1\}$$

1.1.3 Disallowed Transitions

Set:
$$(mm') \in DAL \ \forall t \in T_{minassure}$$

Where
$$(mm')$$
: {(ST, OD), (OD, ST), (CleanSTOD, ST), (CleanODST, OD)}

Constraint:

$$z_{mm',t} = 0 \ \forall (mm') \in DAL \ \forall t \in T_{minassure}$$

1.1.4 Minimal Mode Duration- Correction

Using this inequality we ensure switch is for at least $\theta_{mm'}$ time steps.

$$y_{m',t} \geq \sum_{k=0}^{\theta mm'-1} z_{mm',t-k} \ \forall m,m' \in M, \ \forall t \in T$$

Where $\theta_{mm'}$ is the needed minimal duration of the new mode (a parameter).

1.1.5 Restricting Mode switching as per Pre-Defined Required Intermediate Transitions - Not Present

We have the following set of pre-defied required sequences:

If we denote its elements as: (m,m',m'') The constraint is written as: $z_{mm',t-\theta_{mm'}}-z_{m'm'',t}=0 \ \forall (m,m',m'') \in Seq \ \forall t \in T$

1.2 Process Model

1.2.1 Realising and Bounding the Production rate of Cl_2 based on the active-mode realised using decision variable

The constraint is written as:

$$\underline{\dot{m}}_{Cl_2,m}.y_{m,t} \le \dot{m}_{Cl_2,m,t} \le \bar{\dot{m}}_{Cl_2,m}.y_{m,t} \ \forall m \in M, t \in T$$

Where: (Both active modes are equivalent in terms of production)

$$\begin{array}{ll} \underline{\dot{m}}_{Cl_2,m} = \underline{\dot{m}}_{Cl_2} & m = (ST,OD) \\ \underline{\dot{m}}_{Cl_2,m} = \underline{\dot{m}}_{Cl_2} & m = (ST,OD) \\ \end{array}$$

and

$$\underline{\dot{m}}_{Cl_2,m} = \bar{\dot{m}}_{Cl_2,m} = 0 \ m = \{CleanSTOD, CleanODST\}$$

1.2.2 Total Cl_2 Production

Total production is determined as sum of production rate in each mode as:

$$\dot{m}_{Cl_2,t} = \sum_{m \in M} \dot{m}_{Cl_2,m,t} \ \forall t \in T$$

1.2.3 Production and Consumption of Other Components as per Modes- Not Present

Since, $\dot{m}_{Cl_2,m,t} = 0 \ \forall t \in T$ for cleaning modes i.e. $m = \{CleanSTOD, CleanODST\}$, other components are considered only for active mode set.

Active mode set: $M_{Ac} = (ST, OD)$

Defined separately because of different stoichiometry, can be clubbed in one equation too.

1. NaCl (Consumption in Both Active Modes)

$$\dot{m}_{NaCl,m,t} = \frac{2*M_{NaCl}}{M_{Cl_2}}.\dot{m}_{Cl_2,m,t} \ \forall m \in M_{Ac} \ \forall t \in T$$

2. O_2 Consumption only in OD Mode

$$\dot{m}_{O_2,OD,t} = \frac{M_{O_2}}{2*M_{Cl_2}}.\dot{m}_{Cl_2,OD,t} \ \forall t \in T$$

3. Equivalent H_2 Production in OD Mode (Virtual) to be used as Cost

Since this is what we are buying to meet the downstream demand of H_2 (which is fulfilled in the ST Mode, hence we pay for H_2 while in OD Mode)

$$\dot{m}_{H_2,OD,t} = \frac{M_{H_2}}{M_{H_2}}.\dot{m}_{Cl_2,OD,t} \quad \forall t \in T$$

1.3 Storage Tank

1.3.1 Defining Backup Time

$$S_{Cl_2,t} = \frac{m_{S,Cl_2,t}}{\dot{m}_{N,Cl_2}} \ \forall t \in T \text{ in seconds}$$

1.3.2 Constraining Initial and Final Backup Time

Some same pre-defined value: For Total Production of Cl_2 to just be dependent on productions from mode same.

$$S_{Cl_2,1} = 1hr = 1 * 3600s$$

$$S_{Cl_2,t_n} = 1hr = 1 * 3600s$$

1.3.3 Lower and Upper Bound on Backup-Time

As defined:

$$\underline{S}_{Cl_2} \le S_{Cl_2,t} \le \bar{S}_{Cl_2}$$

$$\bar{S}_{Cl_2} = 3h = 3 * 3600s$$

$$\underline{S}_{Cl_2} = 0h = 0s$$

1.3.4 Connecting Effective Supply, Storage tank and Plant: Overall Mass balance - Not Present

Mass balance is as:

For the equations involving time step index of: (t+1) in them, would yield to error if iterated over $\forall t \in T$. (as also seen in 1.1.2).

This forces us to define another working set w.r.t time steps t. The set should be such as excluding the last element: $t \in T/\{t_n\}$

Thus, we define set $T_{ramp} = \{t_1, t_2, ..., t_{n-1}\}$

$$\dot{m}_{Cl_2,t}\Delta t + m_{S,Cl_2,t} - m_{S,Cl_2,t+1} = \dot{m}_{N,Cl_2}\Delta t \ \forall t \in T/\{t_n\} \ or \ T_{ramp}$$

Demand is satisfied either from the:

- 1. Plant Production: Which is oversized (1.1 times) (to fill/prepare the storage tank for potential future down times and counter the ramping constraint)
- 2. Storage Tank: If No Mode is active, hence, decrease in the Cl_2 mass content.

Note: We would also need storage tank even when there are no cleaning modes in between: Because of the ramping constraint

The constant higher demand won't be satisfied for the initial couple of time steps until the maximum production rate of the particular mode is realised.

Ramping Constraints

Defined maximum allowable increase/decrease $\Delta \dot{m}_{Cl_2}$

The production can be varied between $\underline{\dot{m}}_{Cl_2}$ and $\bar{\dot{m}}_{Cl_2}$ with, $\Delta \dot{m}_{Cl_2} = \frac{\bar{\dot{m}}_{Cl_2} - \underline{\dot{m}}_{Cl_2}}{\theta_{ramp}\Delta t}$

$$\Delta \dot{m}_{Cl_2} = \frac{\dot{m}_{Cl_2} - \underline{\dot{m}}_{Cl_2}}{\theta_{ramp} \Delta t}$$

Thus, depending on the current production rate $\dot{m}_{Cl_2,t}$ at time step t, the maximum and minimum allowable production rate at time step t+1 is given as:

$$\dot{m}_{Cl_2,t+1} \leq \dot{m}_{Cl_2,t} + \sum_{m} y_{m,t} \Delta \dot{m}_{Cl_2} \Delta t + (1 - \sum_{m} y_{m,t}) \underline{\dot{m}}_{Cl_2} \ \, \forall m \in M_{Ac} \ \, \forall t \in T/\{t_n\} \ \, or \ \, T_{ramp}$$

$$\dot{m}_{Cl_2,t+1} \geq \dot{m}_{Cl_2,t} - \sum_{m} y_{m,t+1} \Delta \dot{m}_{Cl_2} \Delta t - (1 - \sum_{m} y_{m,t+1}) \underline{\dot{m}}_{Cl_2} \ \, \forall m \in M_{Ac} \ \, \forall t \in T/\{t_n\} \ \, or \ \, T_{ramp}$$

$$\dot{m}_{Cl_2,t} \geq \sum_{m \in M} y_{m,t} \underline{\dot{m}}_{Cl_2,m} \ \forall t \in T$$

The above constraint has been defined in a way in section 1.2.1.

1.5 Component Expenses

1.5.1 ST Mode

Based on maximum purchase of NaCl:

$$ExpC_{ST,t} \le y_{ST,t} \frac{2*M_{NaCl}}{M_{Cl_2}} \bar{m}_{Cl_2} p_{NaCl} \Delta t \ \forall t \in T$$

Also, based on the actual Cl_2 in that mode,

$$\dot{m}_{NaCl.ST.t}p_{NaCl}\Delta t \leq ExpC_{ST.t} \ \forall t \in T$$

1.5.2 OD Mode

Based on maximum amount of NaCl and O_2 to be purchased. Also, to meet the H_2 demand, the cost of purchasing it from external sources has also been added.

We assume H_2 production to be equivalent to Cl_2 produced.

$$ExpC_{OD,t} \leq y_{OD,t} \left(\frac{2*M_{NaCl}}{M_{Cl_2}} \bar{\dot{m}}_{Cl_2} p_{NaCl} + \frac{M_{O_2}}{2*M_{Cl_2}} \bar{\dot{m}}_{Cl_2} p_{NaCl} + \frac{M_{H_2}}{M_{Cl_2}} \bar{\dot{m}}_{Cl_2} p_{O_2} \right) \Delta t$$

$$(\dot{m}_{NaCl,OD,t} p_{NaCl} + \dot{m}_{O_2,OD,t} p_{O_2} + \dot{m}_{H_2,OD,t} p_{H_2}) \Delta t \leq ExpC_{OD,t} \ \forall t \in T$$

1.5.3 Cleaning Modes

There is no consumption/production in cleaning modes.

$$ExpC_{m,t} = 0 \ \forall m \in M_{clean} = \{CleanSTOD, CleanODST\} \ \forall t \in T$$

1.6 Electricity Demand

1.6.1 Linearising Demand

The demand is NOT Linearly dependent on the Cl_2 production rate: $\dot{m}_{Cl_2,t}$ Thus, the demand is linearised as:

$$P_{m,t} = \sum_{e} (k_{m,e,t}.b_{m,e} + a_{m,e}.\dot{m}_{linCl_2,m,e,t} \frac{3600s}{1h}) \ \forall m \in M, t \in T$$

Define $a_{m,e}$ and $b_{m,e}$ as 0 for the cleaning modes. Thus, then the Demand $P_{m,t}$ will be non-zero only for active modes (thus, no need to have additional constraint for it to be 0).

1.6.2 Defining the Active Interval

Only 1 interval of any 1 mode active mode can be True at a Time Step:

$$\sum_{e \in E} k_{m,e,t} = y_{m,t} \ \forall m \in M, t \in T$$

1.6.3 Correlating Linearised Production rate with Overall Production Rate

As below by following constraints:

$$\dot{m}_{linCl_2,m,e,t} \leq \bar{\dot{m}}_{Cl_2,e}.k_{m,e,t} \ \forall m \in M, t \in T, e \in E$$

$$\dot{m}_{linCl_2,m,e,t} \ge \underline{\dot{m}}_{Cl_2,e}.k_{m,e,t} \ \forall m \in M, t \in T, e \in E$$

Here $\bar{m}_{Cl_2,e}$ is the maximum value of production rate of each interval e, and similarly.

 $\underline{\dot{m}}_{Cl_2,e}$ is the minimum value of production rate of each interval e.

Finally,

$$\sum_{e \in e} \sum_{m \in M} \dot{m}_{linCl_2, m, e, t} = \dot{m}_{Cl_2, t} \ \forall t \in T$$

1.7 Electricity Expenses

Electricity Expense = Mode Demand * Price

1.7.1 ST Mode

The maximum expense is given as:

$$ExpEl_{ST,t} \leq y_{ST,t}(P_{ST,t})_{max}p_{El,t}\Delta t \ \forall t \in T$$

Where, $(P_{ST,t})_{max}$ is maximum y value at the end of interval 2 on x-axis.

$$P_{ST,t}p_{El,t}\Delta t \frac{1}{3600} \le ExpEl_{ST,t} \ \forall t \in T$$

Note: Check units of $(P_{ST,t})_{max}$

1.7.2 OD Mode

Similarly, expense in OD mode is written as:

$$ExpEl_{OD,t} \le y_{OD,t}(P_{OD,t})_{max}p_{El,t}\Delta t \ \forall t \in T$$

Where, $(P_{OD,t})_{max}$ is maximum y value at the end of interval 2 on x-axis for OD line.

$$P_{OD,t}p_{El,t}\Delta t \frac{1}{3600} \le ExpEl_{OD,t} \ \forall t \in T$$

Note: Check units of $(P_{OD,t})_{max}$

1.7.3 Cleaning Modes

 $ExpEl_{m,t} = 0 \ \forall m \in M_{clean} = \{CleanSTOD, CleanODST\} \ \forall t \in T$

1.8 Objective Function

Define total expenses for electricity and components as:

$$ExpEl = \sum_{t} \sum_{m} ExpEl_{m,t} \ \forall m \in M, t \in T$$

$$ExpC = \sum_{t} \sum_{m} ExpC_{m,t} \ \forall m \in M, t \in T$$

Objective = ExpEl + ExpC