



ARTICLE INFO

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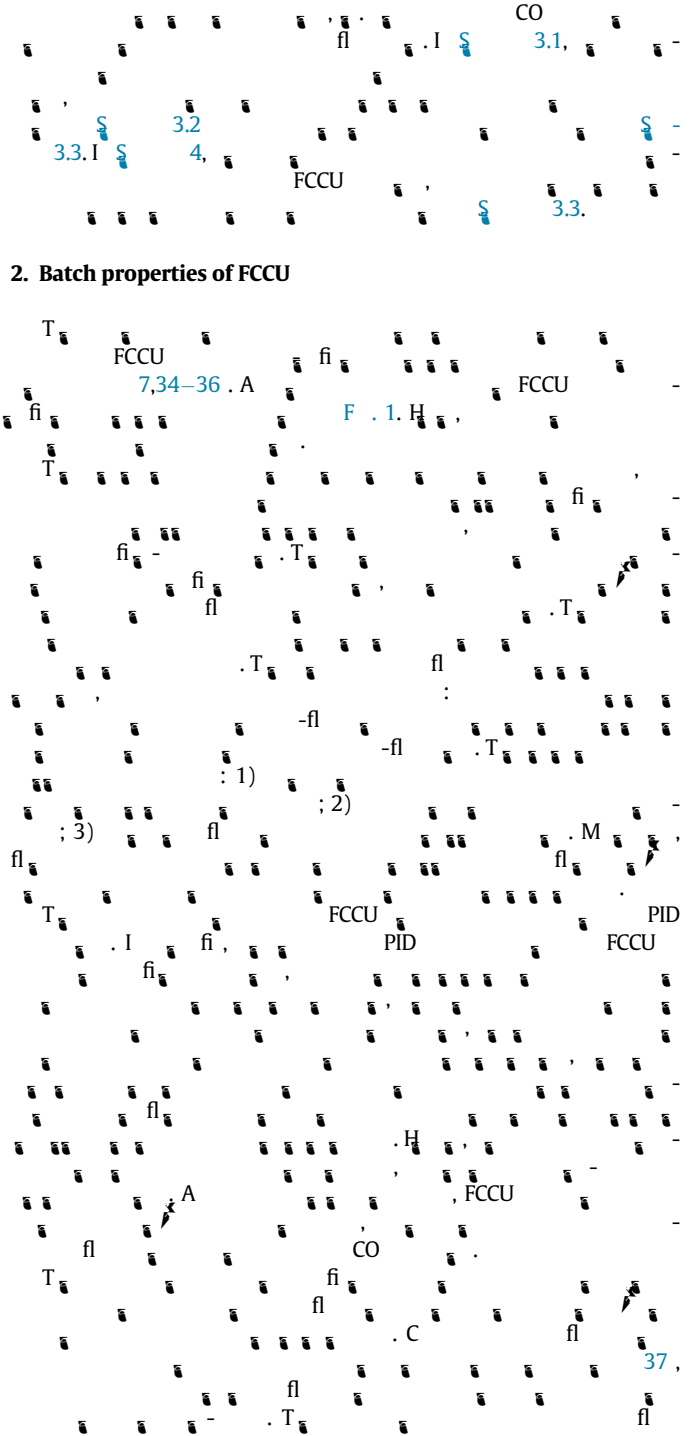
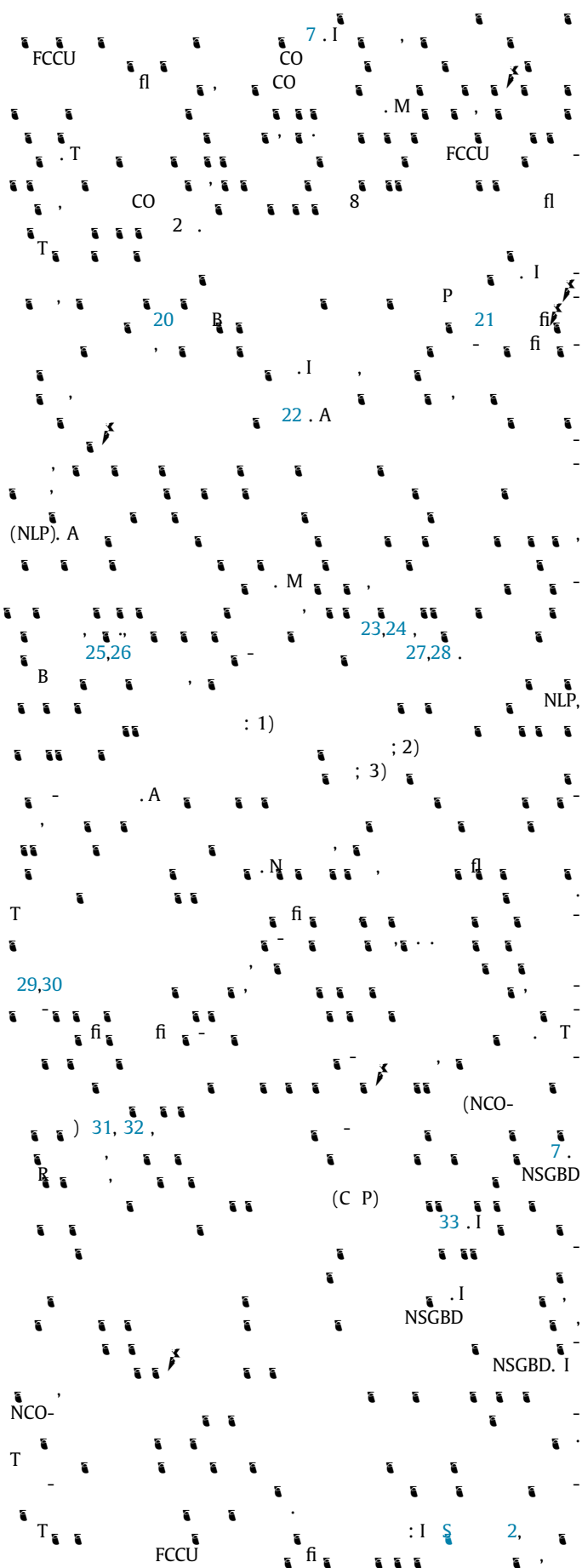
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ABSTRACT

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1. Introduction

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2. Batch properties of FCCU

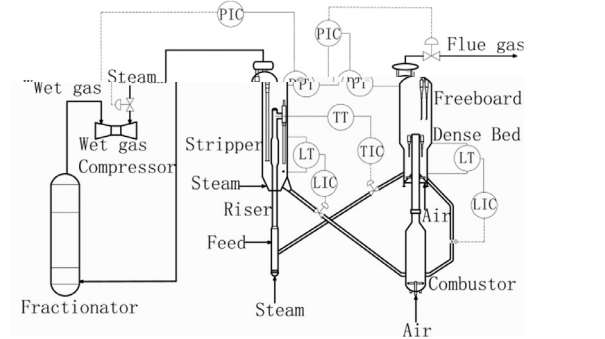
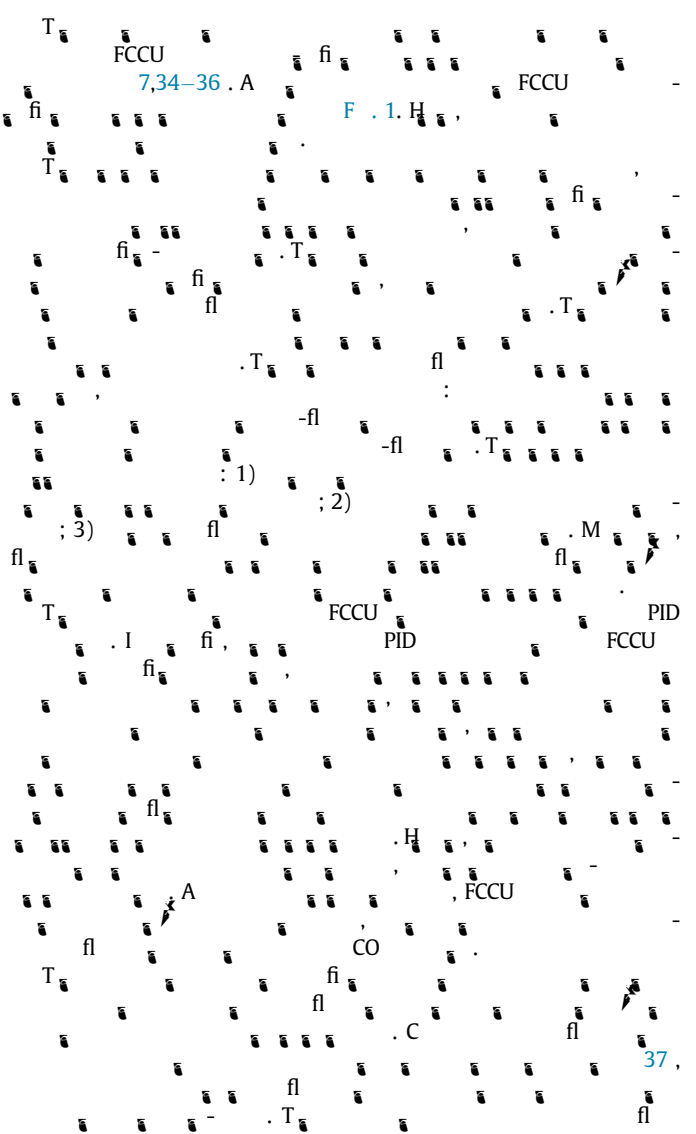
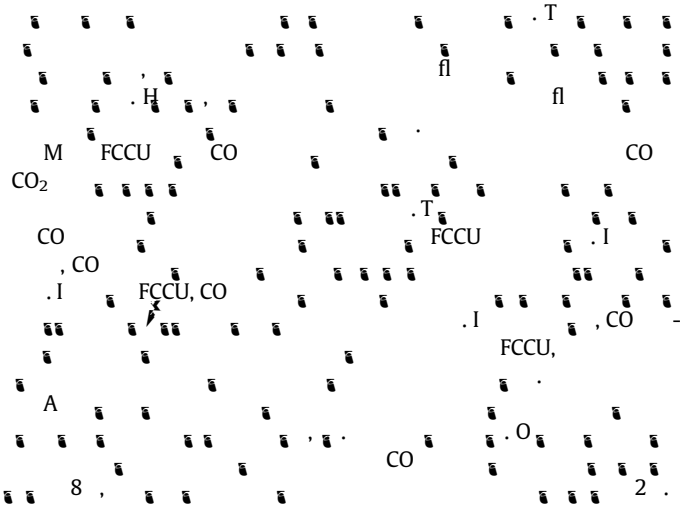


Fig. 1. Schematic diagram of FCCU process components.



$$x_d^{lb} = ((x_d^{lb})^T, (x_a^{lb})^T)^T, x_d^{ub} = ((x_d^{ub})^T, (x_a^{ub})^T)^T, x_d^{lb} \leq x_d \leq x_d^{ub}; u^{lb} \leq u \leq u^{ub} \quad (7)$$

$$x^{lb} \leq x(t_f) \leq x^{ub} \quad (8)$$

$$x_d^{flb} = ((x_d^{flb})^T, (x_a^{flb})^T)^T, x_d^{fub} = ((x_d^{fub})^T, (x_a^{fub})^T)^T, x_d^{flb} \leq x_d \leq x_d^{fub}; u^{flb} \leq u \leq u^{fub} \quad (9)$$

3. Hybrid parametric dynamic optimization

3.1. Mathematical formulation of hybrid parametric dynamic optimization

(DAE):

$$\dot{x}_d = f_d(t, x_d(t), x_a(t), u(t), \bar{u}) \quad (1)$$

$$0 = f_a(t, x_d(t), x_a(t), u(t), \bar{u}) \quad (1)$$

$$J(u(t), \bar{u}) = \int_{t_0}^{t_f} (-r(t, x_d(t), x_a(t), u, \bar{u}) + c_1(t, x_d(t), x_a(t), u, \bar{u})) dt + c_2(\bar{u}) \quad (2)$$

$$\bar{x} = -r + c_1 \quad (3)$$

$$\bar{x}(t_0) = 0 \quad (4)$$

$$u(t), \bar{u} J(x(t_f), \bar{u}) = \bar{x}(t_f) + c_2(\bar{u}) \quad (5)$$

$$x(t) = (x_d(t)^T, x_a(t)^T)^T, x^{lb} \leq x(t) \leq x^{ub} \quad (6)$$

$$u^{lb} \leq u(t) \leq u^{ub} \quad (6)$$

(P1):

$$u(t), \bar{u} J(x(t_f), \bar{u}) \quad (9)$$

$$x_d(t_0) = x_d^0 \quad (9)$$

$$\dot{x}_d = f_d(t, x_d(t), x_a(t), u(t), \bar{u}) \quad (9)$$

$$0 = f_a(t, x_d(t), x_a(t), u(t), \bar{u}) \quad (9)$$

$$G_{\bar{u}}(\bar{u}) \leq 0 \quad (9)$$

$$G_u(u(t)) \leq 0 \quad (9)$$

$$G_p(x(t)) \leq 0 \quad (9)$$

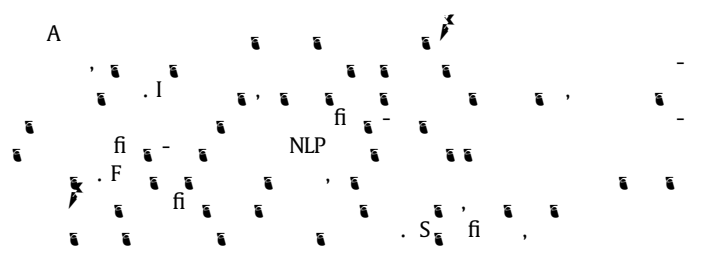
$$G_e(x(t_f)) \leq 0 \quad (9)$$

$$G_{\bar{u}}(\bar{u}) = \begin{pmatrix} \bar{u} - \bar{u}^{ub} \\ \bar{u}^{lb} - \bar{u} \end{pmatrix} \quad (9)$$

$$G_u(u(t)) = \begin{pmatrix} u(t) - u^{ub} \\ u^{lb} - u(t) \end{pmatrix} \quad (9)$$

$$G_p(x(t)) = \begin{pmatrix} x(t) - x^{ub} \\ x^{lb} - x(t) \end{pmatrix} \quad (9)$$

$$G_e(x(t_f)) = \begin{pmatrix} x(t_f) - x^{fub} \\ x^{flb} - x(t_f) \end{pmatrix} \quad (9)$$



$$u(t) \approx \hat{u}^N(t) = \sum_{i=1}^N u_i^N \phi_i^N(t) \quad (10)$$

$$D^N = \{\phi_1^N(t), \phi_2^N(t), \dots, \phi_N^N(t)\}, \quad u_i^N \in \mathbb{R}^m, \quad u(t) \in D, \quad \forall i \neq j, \langle \phi_i^N(t), \phi_j^N(t) \rangle = 0 \quad \forall i \neq j \quad D_N, \quad N \geq 1, \quad t_0 < t_1 < t_2 < \dots < t_N = t_f$$

$$\phi_i^N(t) = \begin{cases} 1, & t_{i-1} \leq t \leq t_i \\ 0, & \text{otherwise} \end{cases} \quad (11)$$

$$\hat{u}_N = ((u_1^N)^T, \dots, (u_N^N)^T)^T \quad \text{NLP. S}$$

$$y^{ub} = y^u + y^b, \quad y^l = y^u - y^b, \quad y^l(t) = y^u(t) - y^b(t), \quad y^l(t_0) = 0, \quad y^u(t_0) = 0, \quad y^l(t_f) = 0, \quad y^u(t_f) = 0. \quad \text{M}$$

$$\hat{u}_N, A \quad \text{NLP} \quad u(t)$$

Problem (P2):

$$\hat{u}_N, \bar{u} J(x(t_f), \bar{u}) \quad (12)$$

$$MX(t_0) = X_0 \quad (12)$$

$$M\dot{X}(t) = F(t, X(t), \hat{u}_N, \bar{u}) \quad (12)$$

$$G(\bar{u}, \hat{u}_N, X(t_f)) \leq 0 \quad (12)$$

$$M = \begin{pmatrix} 1, \dots, 1, 0, \dots, 0 \\ 3n_d + 2n_a & n_a \end{pmatrix} \quad (12)$$

$$X(t) = \begin{pmatrix} x_d(t) \\ x^b(t) \\ x_a(t) \end{pmatrix} \quad (12)$$

$$X_0 = \begin{pmatrix} x_d^0 \\ 0 \\ 0 \end{pmatrix} \quad (12)$$

$$F(t, X(t), \hat{u}_N, \bar{u}) = \begin{pmatrix} f_d(t, x_d(t), x_a(t), \hat{u}_N, \bar{u}^j) \\ f_b(t, x(t)) \\ f_a(t, x_d(t), x_a(t), \hat{u}_N, \bar{u}^j) \end{pmatrix} \quad (12)$$

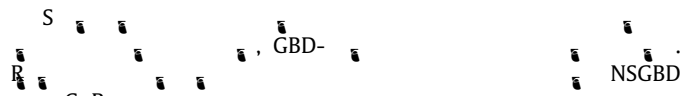
$$f_b(t, x(t)) = \begin{pmatrix} f^x(0, x^{lb} - x(t)) \\ f^x(0, x(t) - x^{ub}) \end{pmatrix} \quad (12)$$

$$G(\bar{u}, \hat{u}_N, X(t_f)) = \begin{pmatrix} G_u(\bar{u}) \\ G'_u(\hat{u}_N) \\ G'_e(x^b(t_f)) \\ G_e(x(t_f)) \end{pmatrix} \quad (12)$$

$$G'_u(\hat{u}_N) = \begin{pmatrix} G_u(u_1^N) \\ \vdots \\ G_u(u_N^N) \end{pmatrix} \quad (12)$$

$$G'_e(x^b(t_f)) = x^b(t_f) \quad (12)$$

3.2. Nonconvex sensitivity-based generalized Benders decomposition



$$: (1) \quad \text{LP}$$

$$; (2)$$

$$; (3)$$

$$\bar{u}, \underline{u}$$

$$h(\bar{u}, \underline{u}) = \underline{u} - \bar{u} = 0 \quad (13)$$

Problem (P3):

$$\hat{u}_N, \bar{u}^j J_a^j = \hat{u}_N J(x(t_f), \bar{u}^j) \quad (14)$$

$$MX(t_0) = X_0 \quad (14)$$

$$M\dot{X}(t) = F(t, X(t), \hat{u}_N, \bar{u}^j) \quad (14)$$

$$G(\bar{u}^j, \hat{u}_N, X(t_f)) \leq 0 \quad (14)$$

Problem (P4):

$$(\hat{u}_N, \bar{u}^j, \mu_a^j) = \hat{u}_N, \bar{u}^j J(x(t_f), \bar{u}) \quad (15)$$

$$MX(t_0) = X_0 \quad (15)$$

$$M\dot{X}(t) = F(t, X(t), \hat{u}_N, \bar{u}) \quad (15)$$

$$G(\bar{u}, \hat{u}_N, X(t_f)) \leq 0 \quad (15)$$

$$h(\bar{u}, \underline{u}_a^j) = 0 \quad (15)$$

$$\mu_a^j \quad (15)$$

Problem (P5):

$$(\hat{u}_{N,c}^j, \hat{u}_c^j) = \min_{\hat{u}_N, \bar{u}} \|\bar{u} - \hat{u}_t^j\|_A^2 \quad (16)$$

$$\dots MX(t_0) = X_0 \quad (16)$$

$$M\dot{X}(t) = F(t, X(t), \hat{u}_N, \bar{u}) \quad (16)$$

$$G(\bar{u}, \hat{u}_N, X(t_f)) \leq 0 \quad (16)$$

$$\|\bar{u} - \hat{u}^j\|_A^2 = (\bar{u} - \hat{u}^j)^T A (\bar{u} - \hat{u}^j) \quad (16)$$

Problem (P6):

$$(\alpha_d^j, \hat{u}_{N,d}^j, \hat{u}_d^j | \mu_b^j) = \min_{\alpha, \hat{u}_N, \bar{u}} \alpha \quad (17)$$

$$\dots MX(t_0) = X_0 \quad (17)$$

$$M\dot{X}(t) = F(t, X(t), \hat{u}_N, \bar{u}) \quad (17)$$

$$G(\bar{u}, \hat{u}_N, X(t_f)) - \alpha e \leq 0 \quad (17)$$

$$h(\bar{u}, \hat{u}_c^j) = 0 \quad (17)$$

$$\mu_b^j \cdot (\underline{u} - \bar{u}^{ub}) \leq 0, i \in K_u \quad (17)$$

$$\mu_c^i \cdot (\underline{u} - \bar{u}^{ub}) \leq 0, i \in K_u \quad (18)$$

$$\mu_d^i \cdot (\underline{u} - \bar{u}^{ub}) \leq 0, i \in K_l \quad (18)$$

$$\mu_c^i = (0, \dots, 0, \underbrace{1, 0, \dots, 0}_{i-1}) \quad \mu_d^i = (0, \dots, 0, \underbrace{-1, 0, \dots, 0}_{i-1})$$

Problem (P7):

$$(\eta_b^k, \underline{u}_b^k | \nu_a^k, \nu_b^k, \nu_c^k, \nu_d^k) = \min_{\underline{u}} \eta \quad (19)$$

$$\eta \geq J_a^j + \mu_a^j \cdot (\underline{u} - \bar{u}_a^j), j \in K_{feas} \quad (19)$$

$$\mu_b^j \cdot (\underline{u} - \bar{u}_c^j) \leq 0, j' \in K_{infeas} \quad (19)$$

$$\mu_c^i \cdot (\underline{u} - \bar{u}^{ub}) \leq 0, i \in K_u \quad (19)$$

$$\mu_d^i \cdot (\underline{u} - \bar{u}^{ub}) \leq 0, i \in K_l \quad (19)$$

$$K_u = \{i \in \{1, \dots, n\} : \nu_c^i \neq 0\} \quad K_l = \{i \in \{1, \dots, n\} : \nu_d^i \neq 0\}$$

$$\Xi_a = \{j \in \{1, \dots, m\} : (\nu_a^j)_j \neq 0\} \quad (20)$$

$$\Xi_b = \{j' \in \{1, \dots, m\} : (\nu_b^j)_{j'} \neq 0\} \quad (20)$$

$$\Xi_c = \{i \in \{1, \dots, n\} : (\nu_c^i)_i \neq 0\} \quad (20)$$

$$\Xi_d = \{i' \in \{1, \dots, n\} : (\nu_d^i)_{i'} \neq 0\} \quad (20)$$

Problem (P8):

$$(\underline{u}_c^k) = \min_{\underline{u}} \mu_a^k \cdot \underline{u} \quad (21)$$

$$\mu_b^j \cdot (\underline{u} - \bar{u}_c^j) \leq 0, j' \in K_{infeas} \quad (21)$$

$$\mu_c^i \cdot (\underline{u} - \bar{u}_i) \leq 0, i \in K_u \quad (21)$$

$$\mu_d^i \cdot (\underline{u} - \bar{u}_i) \leq 0, i' \in K_l \quad (21)$$

$$LBD > UBD \quad (22)$$

$$UBD - LBD < \varepsilon_1 \quad (22)$$

$$\|\mu_a^k / J_a^k\|_B \leq \varepsilon_2 \quad (23)$$

$$\|\underline{u}_b^k - \underline{u}_c^k\|_B \leq \varepsilon_3 \quad (23)$$

Algorithm 1: NSGBD with CVP for Problem (P1)

Step 1. $t_0, t_f, t_0 < t_1 < t_2 < \dots < t_N = t_f$

E . (7); $j = 1, j' = 1, K_{feas} = \emptyset, K_{infeas} = \emptyset, LBD = -\infty;$
 $\gamma, \varepsilon_1, \varepsilon_2, \varepsilon_3.$

Step 2. S $(P3)$ $\bar{u}_a^j = \bar{u}_t^j, O$

(1). P $(P3)$ $\hat{u}_{N,a}^j, J_a^j;$
 P $(P4)$ $\underline{u}_a^j = \bar{u}_a^j, \hat{u}_{N,a}^j, \mu_a^j, UBD = J_a^j; O$

(1). $LBD > UBD, \mu_a^l = \gamma \mu_a^l, l \in \Xi_a.$

(2). $UBD - LBD < \varepsilon_1, O$

(a). $|\Xi_b| + |\Xi_c| + |\Xi_d| = 0 (\bar{u}_a^j)$ $I E . (23)$ $(\hat{u}_{N,a}^j, \bar{u}_a^j),$

$\mu_a^l = \gamma \mu_a^l, l \in \Xi_a.$

(b). $|\Xi_b| + |\Xi_c| + |\Xi_d| \neq 0 (\bar{u}_a^j)$ S P $(\hat{u}_{N,a}^j, \bar{u}_a^j).$

(3). O

$K_{feas} = \{K_{feas}, j\}; j = j + 1.$

(2). P $(P3)$ S P $(P5)$ \bar{u}_t^j
 $(\hat{u}_{N,c}^j, \bar{u}_c^j). S$ P $(P6)$ $\bar{u}_c^j (\hat{u}_{N,c}^j, \bar{u}_c^j) \alpha = 0$

$\mu_b^j \cdot K_{infeas} = K_{infeas}, j' \cdot \bar{u}_t^j = \bar{u}_c^j, j' = j + 1. R$ S $2.$

Step 3. S $(P7)$ $\eta_b^j, \underline{u}_b^j, \nu_a^j, \nu_b^j, \nu_c^j, \nu_d^j;$
 $LBD = \eta_b^j, \bar{u}_t^j = \underline{u}_b^j. R$ S $2.$

Remark 1. T $(P4)$ μ_a^k \bar{u}_a^j $F . 2.$

P $(P3)$ $(P4)$ P $(P3)$ μ_a^k \bar{u}_a^j

P $(P3), P$ $(P5)$ $(P6)$

\bar{u}_c^j $\mu_b^j, \nu_a^j, \nu_b^j, \nu_c^j, \nu_d^j$

$(P5)$ μ_b^j $(P6)$ P $(P5)$

$\alpha = 0. P$ $(P7)$ LP

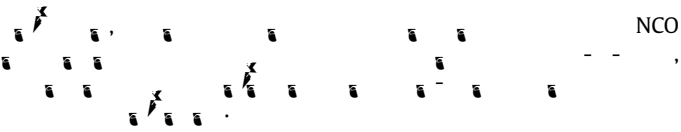
Ξ_a B Ξ_b, Ξ_c Ξ_d

γ LBD Ξ_b, Ξ_c Ξ_d

K_{infeas}, K_u, K_l
 E . (22)
 LBD,
 E . (23) (23)
 P (P8)
 E . (23),
 T NSGBD
 S 2 A 1.
Remark 2. T NSGBD
 : 1) μ_a^j ()
 38 13 $\bar{u}; 2)$
 NSGBD, .

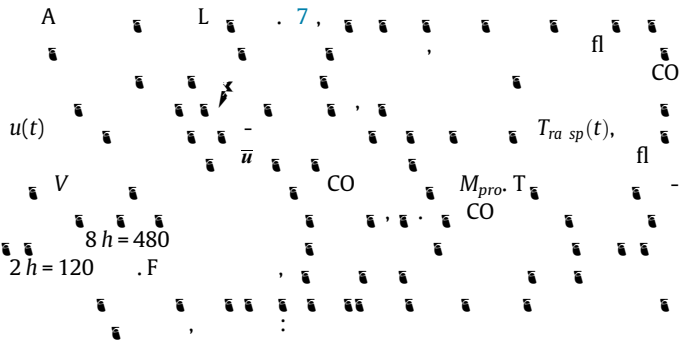
3.3. Novel implementation framework of optimal solution

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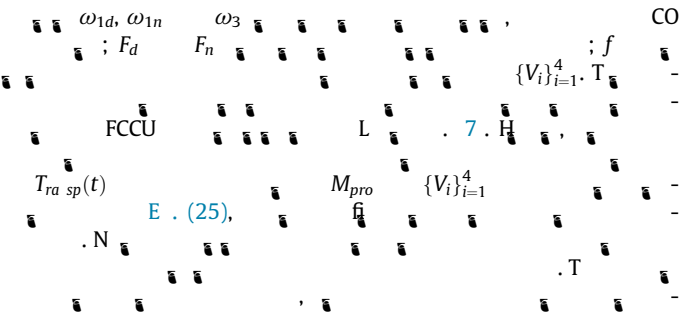


4. Hybrid parametric dynamic optimization of FCCU

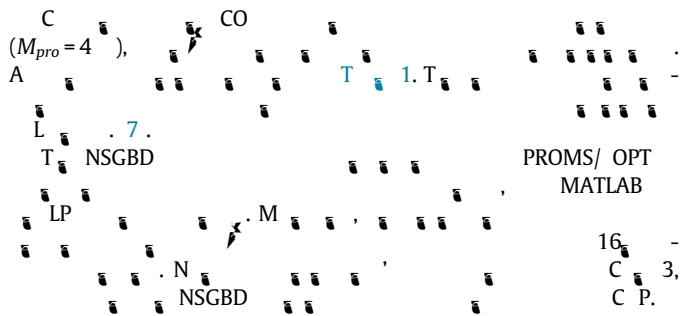
4.1. Mathematical formulation of FCCU



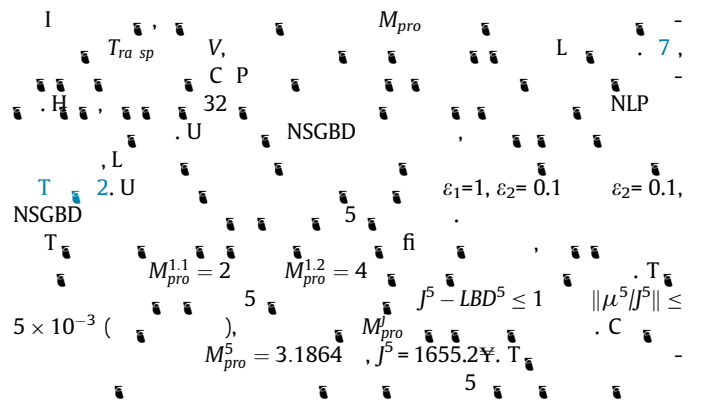
$$J(T_{ra\ sp}(t), \{V_i\}_{i=1}^4, M_{pro}) = \int_0^{480} (-\omega_{1d} F_d(t, T_{ra\ sp}(t), \{V_i\}_{i=1}^4, M_{pro}) - \omega_{1n} F_n(t, T_{ra\ sp}(t), \{V_i\}_{i=1}^4, M_{pro})) dt + \sum_{i=1}^4 \int_{120(i-1)}^{120i} f(V_i) dt + \omega_3 M_{pro} \quad (25)$$



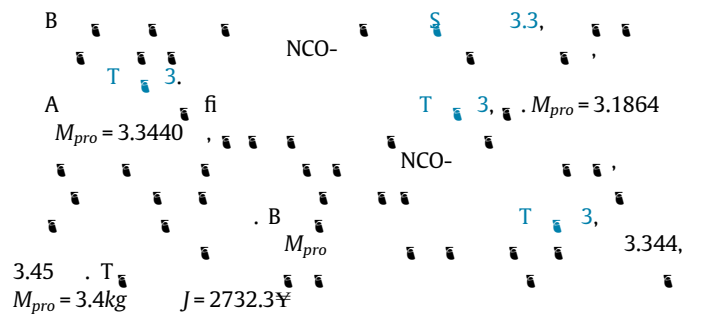
$$J(T_{ra\ sp}(t), V(t), M_{pro}) = \int_0^{480} (-\omega_{1d} F_d(t, T_{ra\ sp}(t), V(t), M_{pro}) - \omega_{1n} F_n(t, T_{ra\ sp}(t), V(t), M_{pro}) + f(V(t))) dt + \omega_3 M_{pro} \quad (26)$$

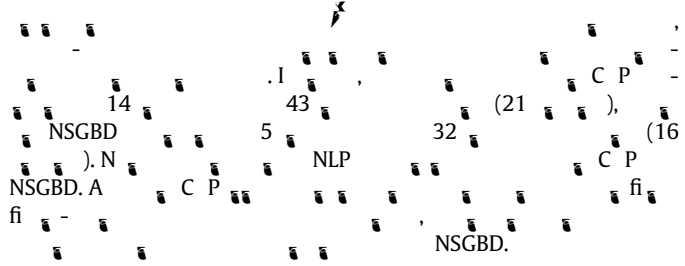
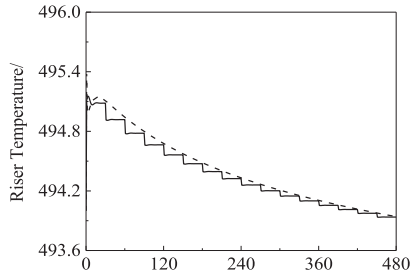


4.2. Case 1: Combustion air as a continuous operation whereas CO promoter as a batch operation



$$M_{pro}^k \in (M_{pro}^k, M_{pro}^k) = (3.1864, 3.3440) \quad (27)$$





4.3. Case 2: Combustion air and CO promoter as batch operations

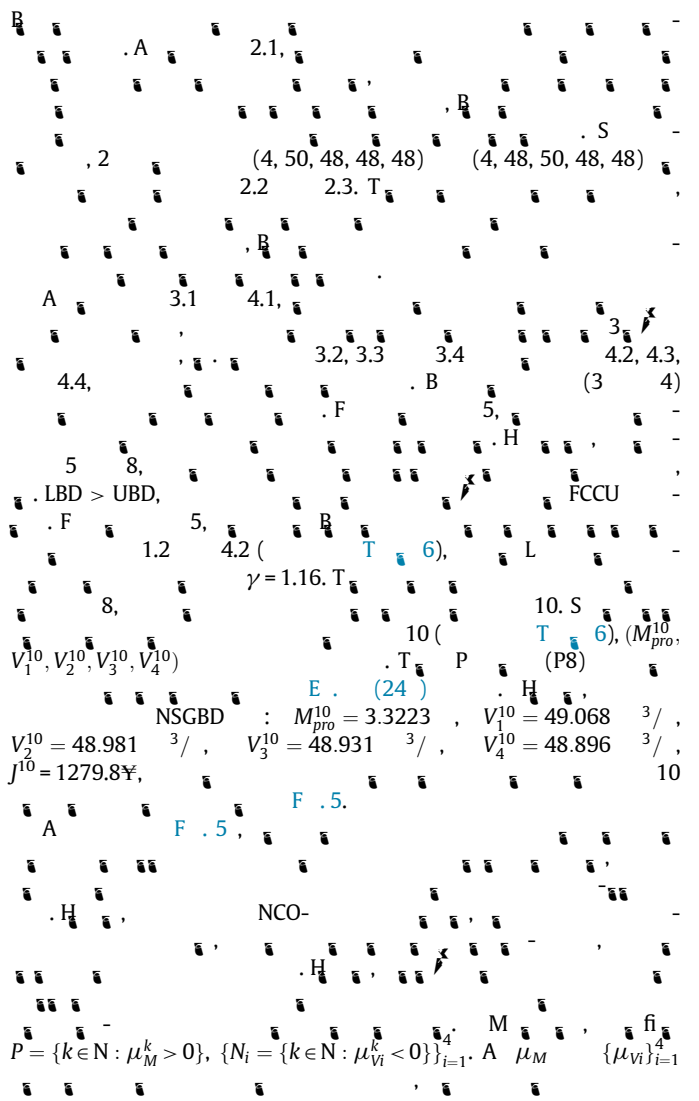
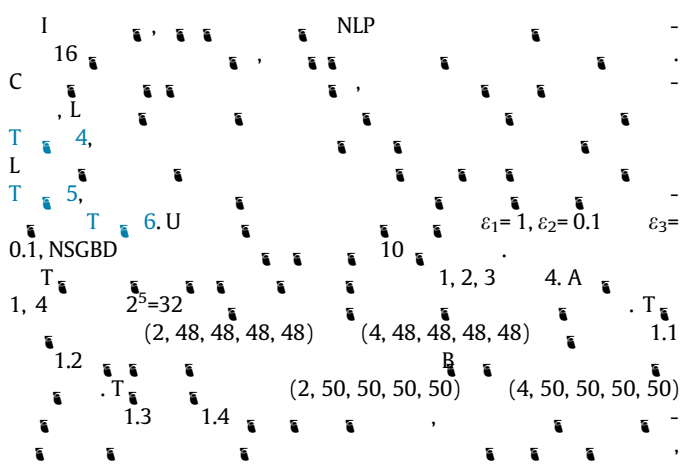


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I_k	4.4	5	6	7	8	9	10
M_{pro} ()	2.5865	2.4590	2.7855	2.8738	2.8890	3.2639	3.3223
μ_M	3461.944	-21.541	27.047	25.754	20.927	53.115	58.887
V_1 ($^3/$)	49.034	49.061	49.064	49.064	49.065	49.068	49.068
μ_{V1}	-3480.3	-3515.4	-3471.9	-3479.8	-3490.8	-3480.0	-3468.3
V_2 ($^3/$)	48.952	48.977	48.978	48.979	48.979	48.980	48.981
μ_{V2}	-3456.5	-3462.7	-3447.1	-3476.1	-3461.9	-3428.1	-3434.2

Ve.(g)1.3(e)-co21 Tf 5.512 0 0 7.6512 154.3181 648.6235 Tm (m)T(53 6.m)Tj 4V4818 0 0 4.25 159.5905 647.5463 Tm (V2)T[(co21 Tf 5. TD (3476.1)Tj /F5 1

$$M_{pro}^* \in (\prod_{k \in P} M_{pro}^k, M_{pro}^{10}) = (2.5865, 3.3223) \quad (28)$$

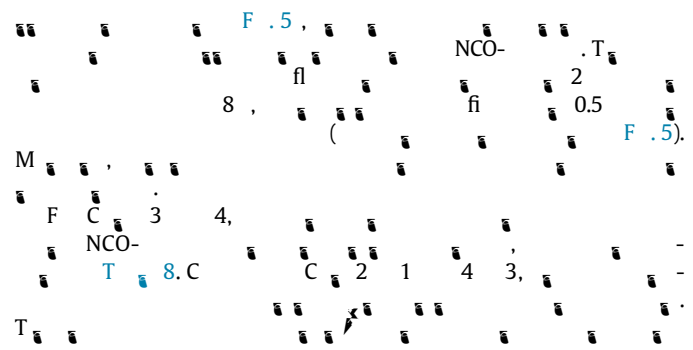
$$V_1^* \in (V_1^{10}, \prod_{k \in N_1} V_1^k) = (49.068, 49.072) \quad ^3/ \quad (28)$$

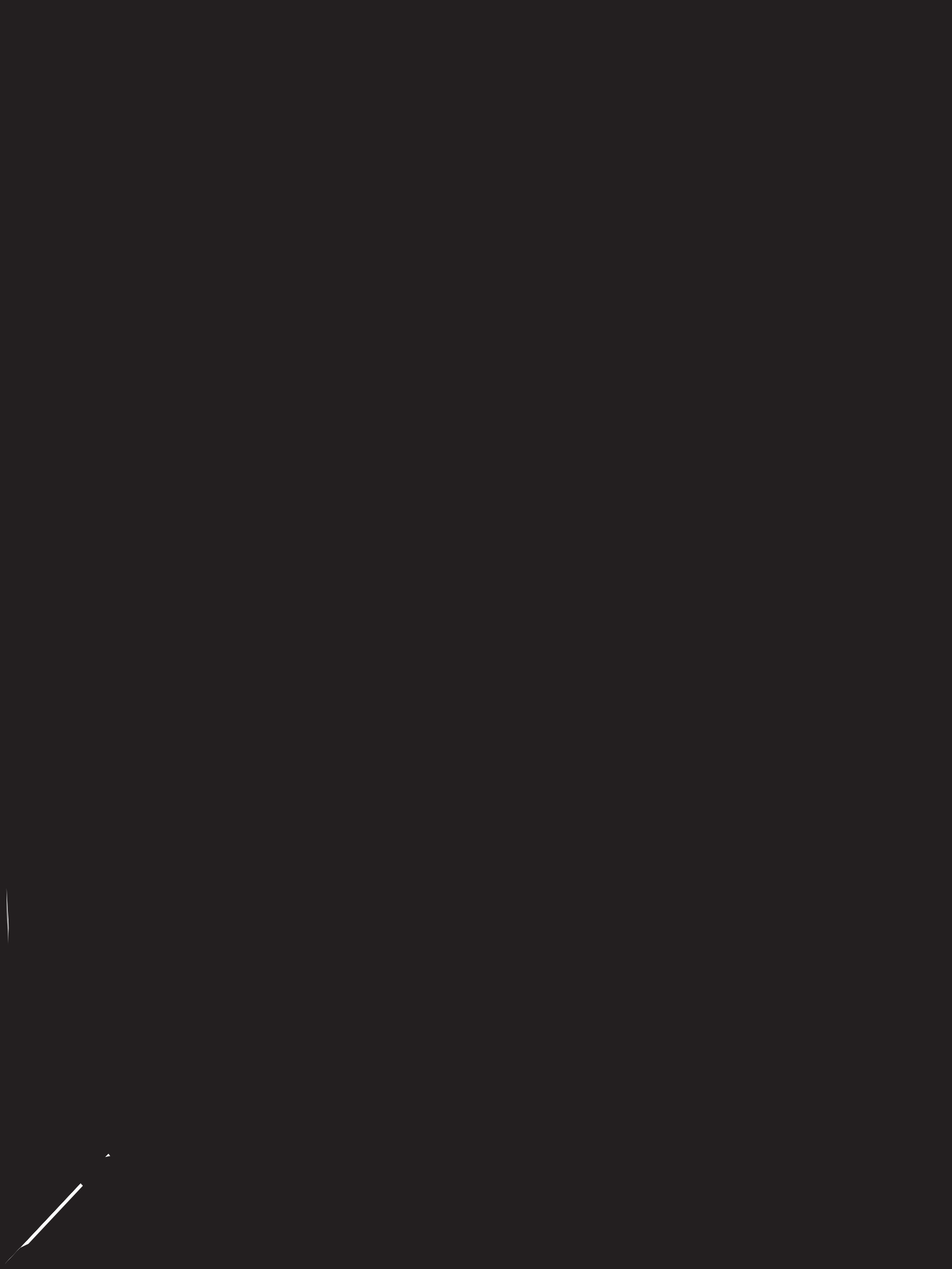
$$V_2^* \in (V_2^{10}, \prod_{k \in N_2} V_2^k) = (48.981, 48.983) \quad ^3/ \quad (28)$$

$$V_3^* \in (V_3^{10}, \prod_{k \in N_3} V_3^k) = (48.931, 48.932) \quad ^3/ \quad (28)$$

$$V_4^* \in (V_4^{10}, \prod_{k \in N_4} V_4^k) = (48.896, 48.897) \quad ^3/ \quad (28)$$

T NCO-
A fi T 7.
($M_{pro}^{10}, V_1^{10}, V_2^{10}, V_3^{10}, V_4^{10}$), T 7.
NSGBD NCO- B
T 7.
: $M_{pro} \in (3.3223, 3.3223)$, $V_1 \in (49.076, 49.080) \quad ^3/$, $V_2 \in (48.988, 48.992) \quad ^3/$, $V_3 \in (48.938, 48.942) \quad ^3/$, $V_4 \in (48.904, 48.908) \quad ^3/$. T
 $M_{pro} = 3.3223$, $V_1 = 49.078 \quad ^3/$, $V_2 = 48.990 \quad ^3/$, $V_3 = 48.940 \quad ^3/$,
 $V_4 = 48.906 \quad ^3/$ J=1890.4¥,
NCO- F .5.A





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