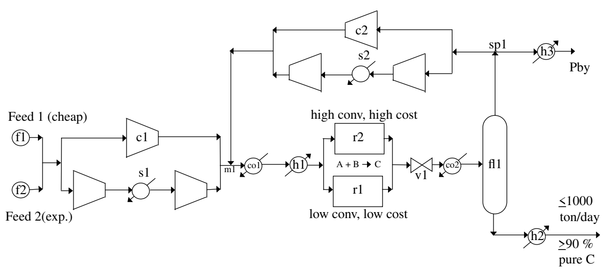
EXAMPLES OF APPLICATION:

☞ The WHEN statement

Synthesis of Process Networks

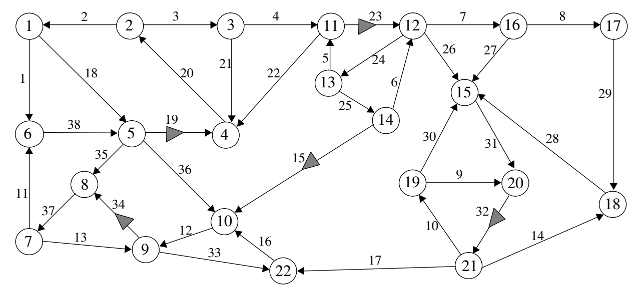


16 alternative configurations embedded in one ASCEND model containing 4 WHEN statements

```
(* Conditional statements *)
     WHEN (select_feed1)
       CASE TRUE:
          USE f1;
       CASE FALSE:
          USE f2;
     END;
     WHEN (select_single1)
       CASE TRUE:
          USE c1;
       CASE FALSE:
          USE s1;
     END;
     WHEN (select_cheapr1)
       CASE TRUE:
          USE r1;
       CASE FALSE:
          USE r2;
     END;
     WHEN (select_single2)
       CASE TRUE:
          USE c2;
       CASE FALSE:
          USE s2;
     END;
```

☞ Complementarity Formulation

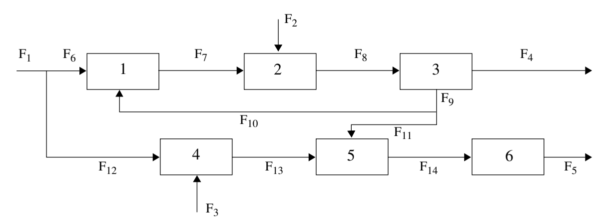
Pipeline Network



$$\begin{bmatrix} H_{ij} = -K \cdot Q_{ij}^2 \\ Q_{ij} \le 0 \end{bmatrix} \vee \begin{bmatrix} H_{ij} = K \cdot Q_{ij}^2 \\ Q_{ij} \ge 0 \end{bmatrix} \qquad \forall arc\ ij\ without\ valve$$

$$\begin{bmatrix} K \cdot Q_{ij}^2 = 0 \\ H_{ij} \le 0 \end{bmatrix} \vee \begin{bmatrix} K \cdot Q_{ij}^2 = H_{ij} \\ H_{ij} \ge 0 \end{bmatrix} \qquad \forall arc\ ij\ with\ valve$$

Linear Mass Balance

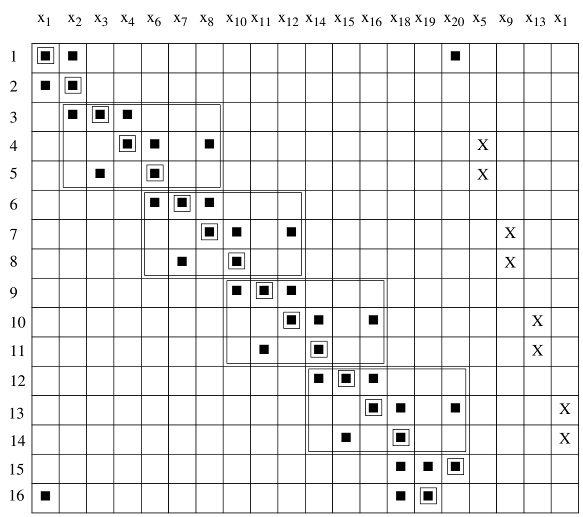


$$\begin{bmatrix} F_6 = 1.1 \cdot F_7 \\ F_{10} = 0.05 \cdot F_7 \\ 0 \le F_7 \le 150 \end{bmatrix} \vee \begin{bmatrix} F_6 = 1.15 \cdot F_7 \\ F_{10} = 0.1 \cdot F_7 \\ 50 \le F_7 \le 80 \end{bmatrix} \vee \begin{bmatrix} F_6 = 1.2 \cdot F_7 \\ F_6 = 0.2 \cdot F_7 \\ 80 \le F_7 \le 150 \end{bmatrix}$$

SOLUTION OF CONDITIONAL MODELS

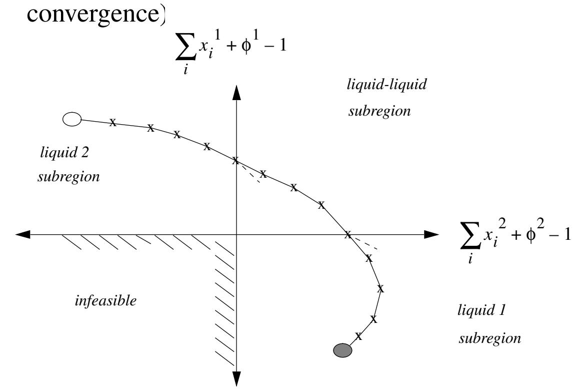
☞ Structural Analysis

- Combinatorial consistency analysis for all of the alternative sets of equations.
  - Common Incidence Pattern
  - Sets of repeated structures



☞ Boundary Crossing Algorithm

- Non-differentiabilities are isolated in boundaries
- Dissection of the feasible region in 2^l subregions
- Inside a subregion use quasi-newton step (quadratic convergence)
- In a boundary use a subgradient method (linear convergence)



☞ Complementarity Formulation

$$\begin{bmatrix}\sum_{i \in C} x_i^2 + \phi^1 < 1 \\ \phi^1 = 0 \\ \eta^2 = 0.5\end{bmatrix} \vee \begin{bmatrix}\sum_{i \in C} x_i^2 + \phi^1 \ge 1 \\ \sum_{i \in C} x_i^2 = 1 \\ \eta^1 = 0.5\end{bmatrix} \Rightarrow \begin{matrix}\phi^1 = h_1 & \sum_{i \in C} x_i^2 = 1 - h_2 \\ \eta^2 = 0.5 + h_3 & \eta^1 = 0.5 - h_4\end{matrix}$$

$$\begin{bmatrix}h_1 = 0 \\ h_3 = 0 \\ h_2, h_4 \ge 0\end{bmatrix} \vee \begin{bmatrix}h_2 = 0 \\ h_4 = 0 \\ h_1, h_3 \ge 0\end{bmatrix}$$

$$\Updownarrow$$

$$\begin{matrix}h_1 \cdot h_2 + h_3 \cdot h_4 = 0 \\ h_1 \cdot h_4 + h_3 \cdot h_2 = 0 \\ h_i \ge 0 \quad i \in [1\ldots4]\end{matrix}$$

Disjunctive set of algebraic equations ⇒ Square Non Linear Problem

- Monotonic functions
- Two disjunctive terms in each disjunction
- Can handle inequality constraints by adding two slacks

NEW MODELING TOOLS:

☞ Logical Relations

```
Phase1, Phase2          IS_A boolean;
CONDITIONAL
    condition1:  SUM(x[1][i], i IN components) + Phi[1] >= 1.0;
    condition2:  SUM(x[2][i], i IN components) + Phi[2] >= 1.0;
END;
Phase1 == SATISFIED(condition1);
Phase2 == SATISFIED(condition2);

(*  The symbol == indicates equality in logical relations  *)
```

☞ SELECT Statement

```
(* Conditional compilation.    Selection variables are constants *)

Phase1,  Phase2                  IS_A boolean_constant;

SELECT  (Phase1,Phase2)
    CASE TRUE,TRUE:    SUM(x[1][i], i IN components) = 1.0;
                       SUM(x[2][i], i IN components) = 1.0;
    CASE TRUE,FALSE:   SUM(x[1][i], i IN components) = 1.0:
                       Phi[2] = 0.0;
    CASE FALSE,TRUE:   SUM(x[2][i], i IN components) = 1.0;
                       Phi[1] = 0.0;
END;
```

☞ WHEN Statement

```
(* Provides flexibility for the configuration of the problem *)

sum1 : SUM(x[1][i], i IN components) = 1.0;
sum2:  SUM(x[2][i], i IN components) = 1.0;
fraction1: Phi[1] = 0.0;
fraction2: Phi[2] = 0.0;

WHEN  (Phase1,Phase2)
    CASE TRUE,TRUE:    USE sum1;
                       USE sum2;
    CASE TRUE,FALSE:   USE sum1;
                       USE fraction2;
    CASE FALSE,TRUE:   USE sum2;
                       USE fraction1;
END;
```

CONDITIONAL MODELING IN ASCEND IV

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GOAL:

Modeling and simulation of conditional models in an equation-based modeling environment (ASCEND IV).

CONDITIONAL MODELING

Alternative set of equations involving a common set of parameters. During the simulation, the model consists of the set of invariant equations and the active set of variant equations.

Example: Liquid-Liquid Equilibrium

CONDITIONAL STATEMENTS

$$\begin{array}{ccccc} \text{Both liquid phases} & & \text{Liquid Phase 1} & & \text{Liquid Phase 2} \\ \begin{bmatrix} \sum_i x_i^1 + \phi^1 \ge 1 \\ \sum_i x_i^2 + \phi^2 \ge 1 \\ \sum_i x_i^1 = 1 \\ \sum_i x_i^2 = 1 \end{bmatrix} & \vee & \begin{bmatrix} \sum_i x_i^1 + \phi^1 \ge 1 \\ \sum_i x_i^2 + \phi^2 < 1 \\ \sum_i x_i^1 = 1 \\ \phi^2 = 0 \end{bmatrix} & \vee & \begin{bmatrix} \sum_i x_i^1 + \phi^1 < 1 \\ \sum_i x_i^2 + \phi^2 \ge 1 \\ \phi^1 = 0 \\ \sum_i x_i^2 = 1 \end{bmatrix} \end{array}$$