**MINLP formulation of the reactor network example**

|  |  |  |
| --- | --- | --- |
| *Set of components (index )*  *Set of units in the superstructure (index )* | | (18.A)  (18.B) |
| *Existence of an unreacted feed in unit*  *If There is unreacted feed in reactor*  *Existence of recycle flow in unit*  *If There is recycle in reactor* | (19.A)  (19.B) | |
| *Unit operation in*    *If unit is a CSTR* | (20) | |

|  |  |
| --- | --- |
| *The unit must be a CSTR to include a recycle at* | (21.A) |
| *There is only one unreacted feed* | (21.B) |
| *There is only one recycle stream* | (21.C) |
| *Unreacted feed unit: Partial mole balance* | (21.D) |
| *Unreacted feed unit: Continuity* | (21.E) |
| *Unreacted feed unit: Reaction rates* | (21.F) |
|  | (21.G) |
| *Reactor Sequence: Partial mole balance* | (21.H) |
| *Reactor Sequence: Continuity* | (21.I) |
| *Reactor Sequence: Reaction rates* | (21.J) |
|  | (21.K) |
| *Splitting point: Partial mole balance* | (21.L) |
| *Splitting point: Continuity* | (21.M) |
| *Splitting point: Additional constraints* | (21.N) |
| *Product specification constraint* | (21.O) |
| *Volume constraint* | (21.P) |
| *Objective Function: Total reactor network volume* | (21.Q) |

**GDP formulation of the reactor network example**

|  |  |  |
| --- | --- | --- |
| *Set of components (index )*    *Set of units in the superstructure (index )* | | (18.A)  (18.B) |
| *Existence of an unreacted feed in unit*  *If There is unreacted feed in reactor*  *Existence of recycle flow in unit*  *If There is recycle in reactor* | (19.A)  (19.B) | |
| *Unit operation in :* If at the current unit **every** unit after it (from to ) **is not** an unreacted feed **or** if the current unit has the unreacted feed, then the unit is a CSTR (the opposite is also true)  *If unit is a CSTR, if unit is a bypass* | (20) | |

|  |  |
| --- | --- |
| *The unit must be a CSTR to include a recycle at* | (21.A) |
| *There is only one unreacted feed* | (21.B) |
| *There is only one recycle stream* | (21.C) |
| *Unreacted feed unit* | (21.D-21.G) |
| *Reactor Sequence* | (21.H-21.K) |
| *Splitting point: Partial mole balance* | (21.L) |
| *Splitting point: Continuity* | (21.M) |
| *Splitting point: Additional constraints* | (21.N) |
| *Product specification constraint* | (21.O) |
| *Volume constraint* | (21.P) |
| *Objective Function: Total reactor network volume* | (21.Q) |

**External variables reformulation using GDP**

|  |  |
| --- | --- |
| *External Variables Reformulation* | (22.A)  (22.B)  (22.C)  (22.D)  (22.E) |

**Notes**

* Those Boolean variables that cannot be reformulated can either: 1) stay in the lower level problems or 2) Move to the upper layer and treat those Boolean variables as external variables without reformulation (This (2) is expected to work for problems with few Boolean variables that cannot be reformulated. If any of the Boolean variables is reformulated and every Boolean variable is moved to the upper layer, this would be equivalent to a complete enumeration. 1) would be recommended if many Boolean variables remain without reformulation).
* Note that the reformulation with external variables allows to be calculated in the upper layer, thus the resulting problems are NLP.
* In this case, the external variable’s reformulation can be applied because and satisfy:

But the requirement is more general. Fore example, we have seen we can use this to locate multiple reactive sections. Also, the reformulation should allow to allocate things in multidimensional grids, but I do not know yet how to write this mathematically.