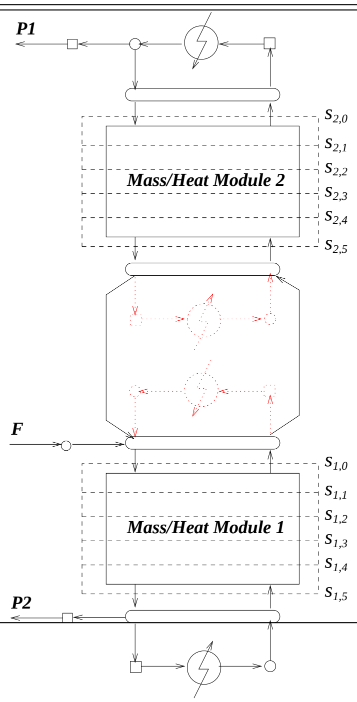
Appendix C

Enhanced GMF Physical Model

C.1 GMF/OC Distillation Column Degrees Of Freedom

The GMF/OC representation of a simple distillation column along with the Structural Sets and assigned binary variables are shown in Table C.1. The GMF/OC equality constraints are enumerated, based on the GMF model statistics provided in Appendix A.5. The placement of the *substituting* and

Table C.1: GMF/OC Structural Data for a Simple Distillation Column

GMF/OC Representation	Structural Sets	Binary Variables
	$E^E = \{1,2\}$	$y_1 = y_2 = 1$
	$E^{HE} = \{1\}$	$y_1^H = 1$
	$E^{CE} = \{2\}$	$y_2^C = 1$
	$I = \{F\}$	$y_{1,1}^{HV} = y_{2,2}^{LH} = 1$
	$C = \{Benz., Tolu.\}$	$y_{2,2}^{VC} = y_{2,2}^{CL} = 1$
	$P = \{P1, P2\}$	
	$E_F^{FL} = \{1\}$	$y_{F,1}^{FL} = 1$
	$E_2^{LLo} = \{1\}\,,\ E_1^{LLi} = \{2\}$	$y_{2,1}^{LL} = 1$
	$E_1^{VVo} = \{2\}\,,\ E_2^{VVi} = \{1\}$	$y_{1,2}^{VV} = 1$
	$E_2^{CLo} = \{2\}\,,\ E_2^{CLi} = \{2\}$	$y_{2,2}^{CL} = 1$
	$E_1^{LPo} = \{P2\}\,,\ E_{P2}^{LPi} = \{1\}$	$y_{1,P2}^{LP} = 1$
	$E_2^{CPo} = \{P1\}\,,\ E_{P1}^{CPi} = \{2\}$	$y_{2,P1}^{CP} = 1$

supplementary constraints is marked with a † and a ‡.

Model Equations

Feed Splitters	$2(I)$
Upper Auxiliary Block	$(4E^{E}+2E^{E}C)$
M/H Main Block †	$(3NC+2NC\,C+4C+8)E^{E}$
Lower Auxiliary Block	$(4E^{E}+2E^{E}C)$
Cooler Module	$(4E^{CE}+E^{CE}C)$
Heater Module	$(4E^{HE}+E^{HE}C)$
Product Mixers	$(3P+P\,C)$
Enthalpy Definitions ‡	$[I+(8+2NC)E^{E}+2E^{HE}+2E^{CE}+P]$
Equil. Const. Definitions ‡	$[I+(6+NC)E^{E}+2E^{HE}+2E^{CE}+P]\,C$
Module Pressure Spec	(E^{E})
Reflux Ratio Definition	(1)
Distillate Purity Spec	(1)
Trays Per M/H module ‡	(E^{E})
Total:	$E^{E}(5NC+3NC\,C+14C+26)+(E^{CE}+E^{HE})(3C+6)+P(2C+4)+I(C+3)+2$

Model Variables

Flowrates ‡	$[(6+2NC)E^{E}+E^{CE}+E^{HE}+P]$
Component Flowrates ‡	$(2NC\,E^{E}+2E^{E})C$
Molar Fractions	$(6E^{E}+E^{CE}+E^{HE}+P)C$
Temperatures ‡	$[I+(8+NC)E^{E}+2E^{CE}+2E^{HE}+P]$
Heater Duty	(E^{HE})
Cooler Duty	(E^{CE})
Enthalpies ‡	$[I+(8+2NC)E^{E}+2E^{CE}+2E^{HE}+P]$
Equilibrium Constants ‡	$[I+(6+NC)E^{E}+2E^{CE}+2E^{HE}+P]C$
M/H module Pressure	(E^{E})
Reflux Ratio	(1)
Interconnection Flowrates	(9)
M/H Module Trays ‡	(E^{E})
Total:	$E^{E}(5NC+3NC\,C+14C+24)+(E^{CE}+E^{HE})(3C+6)+P(2C+3)+I(C+2)+10$

† GMF/OC additional variables:

Flowrates (Liquid and Vapour) $(f^{L}_{e,j},\ f^{V}_{e,j})$: $2(NC+1)E^{E}$

Component Flowrates (Liquid and Vapour) $(fc^{L}_{e,j,c},\ fc^{V}_{e,j,c})$: $2(NC+1)E^{E}C$

Temperatures $(T_{e,j})$: $(NC+2)E^{E}$

Enthalpies (Liquid and Vapour) $(H^{L}_{e,j},\ H^{V}_{e,j})$: $2(NC+1)E^{E}$

Equilibrium Constants $(K_{e,j,c})$: $NCE^{E}C$

Trays of M/H modules (M_{e}): E^{E}

It must be noted that for presentational simplicity throughout this section nc_e has been assumed the same for all M/H modules and replaced by *NC*. The equality constraints for the collocation point locations and weighting functions were incorporated in the balances. Moreover, for the optimization problem of Section 6.5.1 (where *C=2*, E^E*=2*, E^{CE}*=*E^{HE}*=1*, *P=2*, *I=1* and *NC=4*) the number of trays per *M/H* module (M_e) was assumed fixed, eliminating (E^E) degrees of freedom. Therefore, the GMF/OC generated *244* variables and *243* equality constraints, thus leaving the reflux as the single degree of freedom to be optimized for the fixed design problem.

C.2 GMF/OCFE Distillation Column Degrees Of Freedom

Below, † and ‡ mark the locations of *substituting* and *supplementary* information, respectively.

Model Equations

Feed Splitters	*2(I)*
Upper Auxiliary Block	$(4E^E+2E^E C)$
M/H Main Block †	$[(3NC+2NC\,C+2C+4)L+2C+4]E^E$
Lower Auxiliary Block	$(4E^E+2E^E C)$
Cooler Module	$(4E^{CE}+E^{CE} C)$
Heater Module	$(4E^{HE}+E^{HE} C)$
Product Mixers	$(3P+P\,C)$
Enthalpy Definitions †	$[I+(6+2L\,NC+2L)E^E+2E^{HE}+2E^{CE}+P]$
Equil. Const. Definitions †	$[I+(6+L\,NC)E^E+2E^{HE}+2E^{CE}+P]\,C$
Module Pressure Spec	(E^E)
Reflux Ratio Definition	*(1)*
Distillate Purity Spec	*(1)*
Summation of Trays Per M/H module †	(E^E)
Sum:	$E^E[(5NC+3NC\,C+2C+6)L+12C+20]+(E^{CE}+E^{HE})(3C+6)+P(2C+4)+I(C+3)+2$

Model Variables

Flowrates ‡	$[(4+2L\,NC+2L)E^E+E^{CE}+E^{HE}+P]$
Component Flowrates ‡	$(2E^E NC\,L+2E^E L)C$
Molar Fractions	$(6E^E+E^{CE}+E^{HE}+P)C$
Temperatures ‡	$[I+(6+L\,NC+2L)E^E+2E^{CE}+2E^{HE}+P]$
Heater Duty	(E^{HE})
Cooler Duty	(E^{CE})
Enthalpies ‡	$[I+(6+2L\,NC+2L)E^E+2E^{CE}+2E^{HE}+P]$
Equilibrium Constants ‡	$[I+(6+L\,NC)E^E+2E^{CE}+2E^{HE}+P]C$
M/H module Pressure	(E^E)
Reflux Ratio	*(1)*
Interconnection Flowrates	*(9)*
M/H Module Trays	$(E^E L)$
Sum:	$E^E[(5NC+3NC\,C+2C+7)L+12C+17]+(E^{CE}+E^{HE})(3C+6)+P(2C+3)+I(C+2)+10$

† GMF/OCFE additional variables:

Flowrates (Liquid and Vapour) ($f^L_{e,l,j},\ f^V_{e,l,j}$): $2(NC+1)E^E L$

Component Flowrates (Liquid and Vapour) ($fc^L_{e,l,j,c},\ fc^V_{e,l,j,c}$): $2(NC+1)E^E L\,C$

Temperatures ($T_{e,l,j}$): $(NC+2)E^E L$

Enthalpies (Liquid and Vapour) ($H^L_{e,l,j},\ H^V_{e,l,j}$): $2(NC+1)E^E L$

Equilibrium Constants ($K_{e,l,j,c}$): $NC\ E^E L\ C$

Trays of M/H modules ($M_{e,l}$): $E^E L$

The GMF/OCFE equality constraints and variables were enumerated, based on the GMF statistics of Appendix A.5. For presentational simplicity in the above enumeration, L_e is used as its cardinality, $|L_e|$, and it has been assumed the same for all M/H modules (which is in accord with the examined GMF/OCFE case studies) and replaced by L. For the examined problem of Section 6.5.2, where C=2, E^E=2, E^{CE}=E^{HE}=1, P=2, I=1, L=2 and NC=2, the GMF/OCFE generated *266* variables. The number of equality constraints was found equal to *263* (incorporating the equations for the collocation point locations and weighting functions in the balances), thus leaving the reflux and the tray number of one finite element per *M/H* module, as the *3* degrees of freedom for the fixed design optimization problem. The additional *2* degrees of freedom were due to that fact that although the overall number of trays per *M/H* module was known, the boundaries of the Finite Elements could not be specified *a-priori*.