Digital Supplementary Information

Table 1: Process-related constraints.

Constraint	Description
$\boldsymbol{P_{evap.}} \geq 1\ \boldsymbol{atm}$	Evaporator pressure must be greater than 1 atm to prevent vacuum operations.
$P_{con.} \geq P_{evap.} + 0.2$	Condenser pressure must be at least 0.2 bar above evaporator pressure.
$T_{con.\ out} \geq T_{sink} + 5$	The condenser outlet temperature must be at least 5K above the sink temperature.
$T_{evap.\ out} + 5 \leq T_{source}$	The evaporator outlet temperature must be at least 5K below the source temperature.
$T_{con.\ out} \geq T_{evap.\ in}$	The condenser outlet temperature must be greater than or equal to the evaporator inlet temperature. This is a redundant constraint that helps to guide the numerical solver.
$T_{evap.\ in} \geq T_{b\ norm.}$	The evaporator inlet temperature must be greater than the normal boiling temperature. This is a redundant constraint that helps to guide the numerical solver.
$P_{r,\ con.} \leq 0.7$	The reduced pressure in the condenser must be less than or equal to 0.7
$\Delta T_{super.} \leq 100$	Maximum evaporator superheat is 100 K.
$\Delta T_{sub.} \leq 100$	Maximum condenser subcool is 100 K.
$1.2 \leq P_{cond.} \leq 145$	Upper and lower bounds for condenser pressure.
$1.0 \leq P_{evap.} \leq 80$	Upper and lower bounds for evaporator pressure.

Table 2: Initial values for the decision variables.

Decision variable	Initial value	Type
P_c	1.2 bar	Continuous
$\Delta T_{sub.}$	0	Continuous
P_e	1 bar	Continuous
$\Delta T_{super.}$	0	Continuous
a	0	Integer
n	Propane	Integer vector

Table 3: Best benchmark for VHC at each source-sink temperature pair

Best benchmark for VHC		T_{source} (K)				
		340	360	380	400	420
T_{sink} (K)	360	Ammonia **2.39**	-	-	-	-
	380	Ammonia **2.06**	Ammonia **2.98**	-	-	-
	400	1,1,1,3,3-Pentafluoropropane **0.26**	1,1,1,3,3-Pentafluoropropane **0.44**	1,1,1,3,3-Pentafluoropropane **0.73**	-	-
	420	Pentane **0.12**	Pentane **0.21**	Pentane **0.36**	Pentane **0.51**	-
	440	No solution **N/A**	Pentane **0.12**	Water **0.24**	Pentane **0.43**	Pentane **0.70**