



Cycle and component modeling



Cycle analysis

- System models that are used to:
 - Estimate and optimize overall system performance
 - Trade cost and performance
 - Provide boundary conditions for components
 - Evaluate operability
 - Design and optimize controls

Cycle model basics

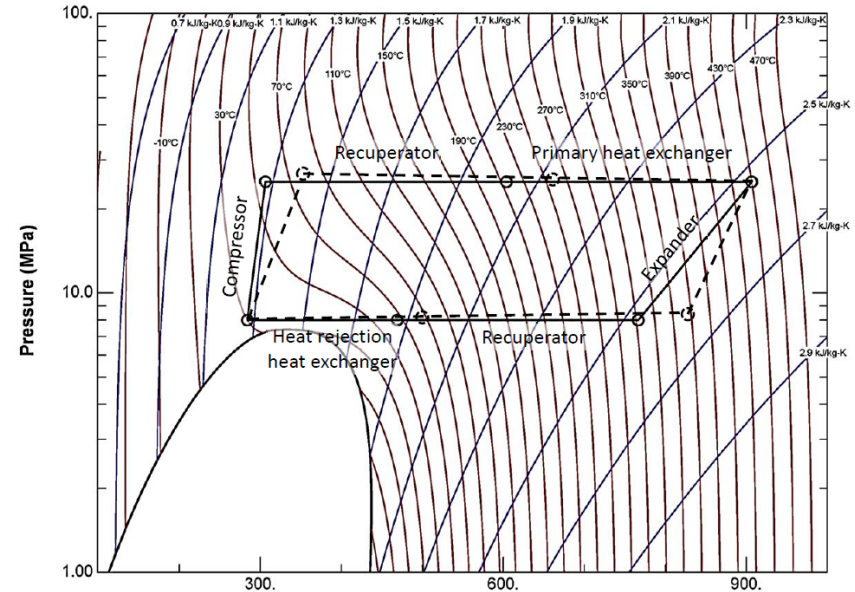
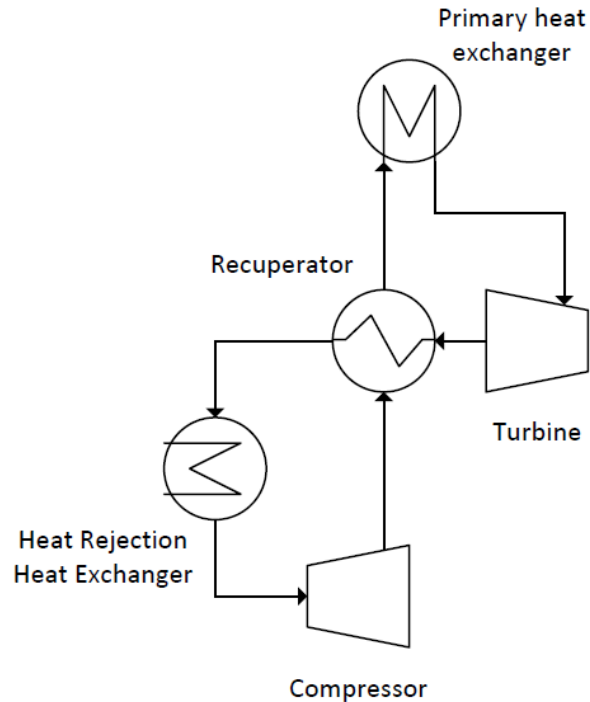
- Fundamental tool to predict performance of a collection of components in a thermodynamic system
- Main principles
 - Conserve mass and energy
 - Define the components with adequate detail
 - Constrain the solution appropriately
 - If $N_{\text{var}} = N_{\text{DOF}}$, you are solving for a single unique solution
 - If $N_{\text{var}} > N_{\text{DOF}}$, you are solving a non-linear optimization problem

Optimization problems are the norm – usually performance and/or cost

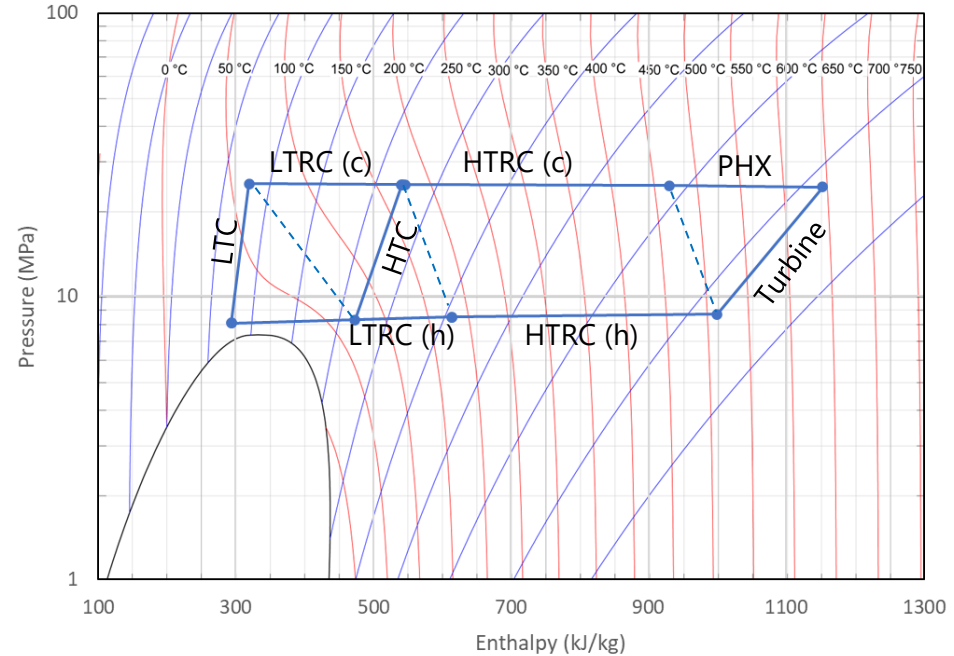
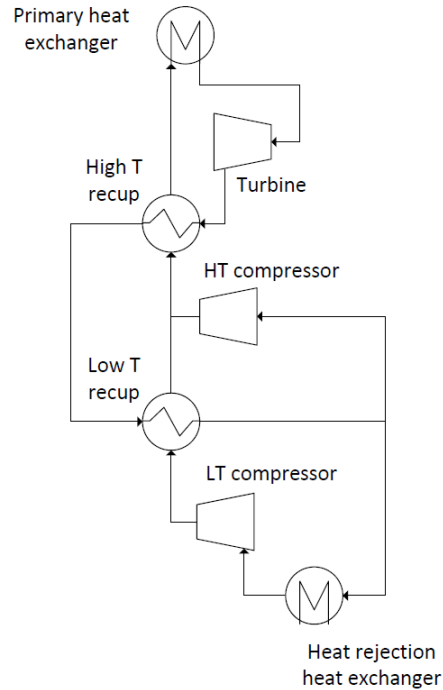
Design models vs performance models

- Design model
 - Boundary conditions (e.g. heat source, heat sink) known at design point
 - Objective: Find arrangement of components that produces some form of optimal outcome
 - Performance
 - Cost
 - Other constraints (e.g. footprint, max P)
- Performance model
 - BCs cover range of values
 - Objective: With a given arrangement of fixed components, find optimal operating state of machine

Example of a closed-loop cycle & components



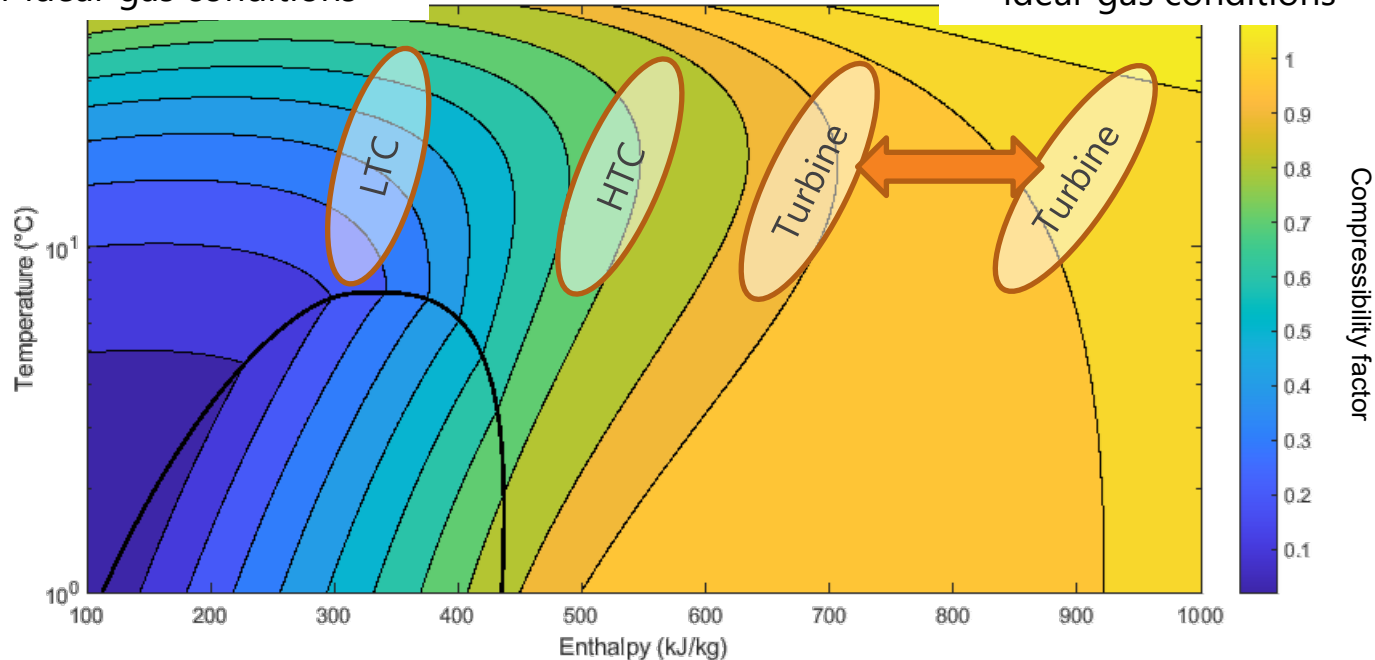
RCB cycle designed for recirculated heat applications with low ΔT



Component operating conditions affect how you model them

Compressors operate in highly non-ideal-gas conditions

Turbines operate in near ideal-gas conditions



Compressor & turbine modeling

- Design mode
 - Inputs:
 - Pressure ratio
 - Flow rate
 - Inlet conditions
 - Isentropic (or polytropic) efficiency
 - Outputs
 - Shaft work
 - Discharge conditions
- Performance mode
 - Inputs:
 - Compressor map
 - Inlet conditions
 - Speed
 - Outputs
 - Shaft work
 - Discharge conditions

Compressor in cycle design mode

- Know : p_1, T_1, p_2 and \dot{m}
 - $h_{2s} = h(p_2, s_1)^*$
 - $h_2 = h_1 + \frac{h_{2s} - h_1}{\eta_s}$
 - $T_2 = T(h_2, p_2)$
 - $W = \dot{m}(h_1 - h_2)$
- Compressor efficiency is an assumption – needs to be consistent with capability

Turbine in cycle design mode

- Know : p_1, T_1, p_2 and \dot{m}
 - $h_{2s} = h(p_2, s_1)$
 - $h_2 = h_1 - \eta_s(h_{2s} - h_1)$
 - $T_2 = T(h_2, p_2)$
 - $W = \dot{m}(h_1 - h_2)$
- Turbine efficiency is an assumption – needs to be consistent with capability

Polytropic vs isentropic efficiency

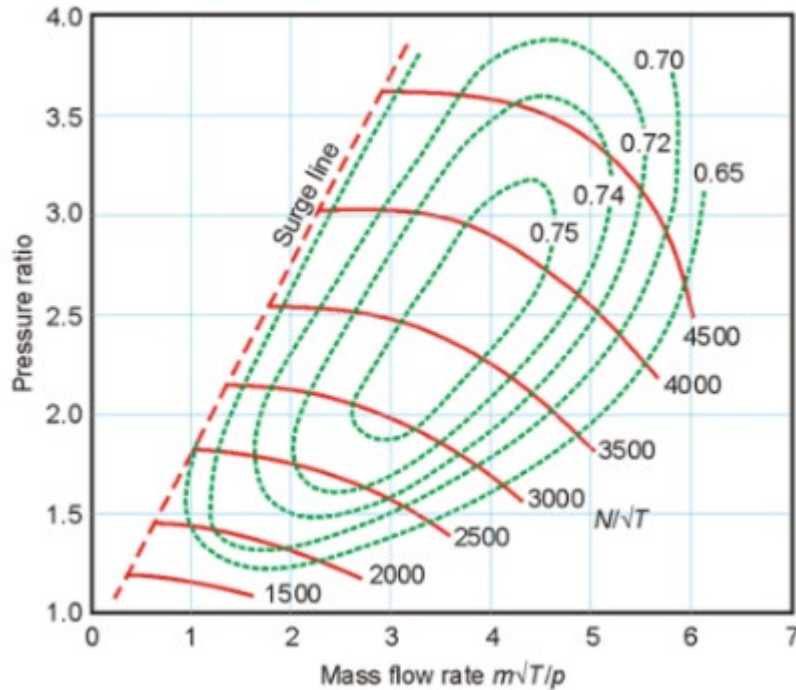
- Thermodynamics & cycle modeling wants isentropic efficiency
- Compressor designers talk in “polytropic efficiency” (efficiency for an incremental change in pressure)
- Can convert between them:

$$\eta_s = \frac{1 - PR^{\eta_p \frac{\gamma-1}{\gamma}}}{1 - PR^{\frac{\gamma-1}{\gamma}}}$$

but what do you use for γ when your fluid is not an ideal gas?

(hint, it's not $\frac{c_p}{c_v}$)

Compressor performance modeling – maps



Given inlet conditions and speed, can output pressure ratio and efficiency

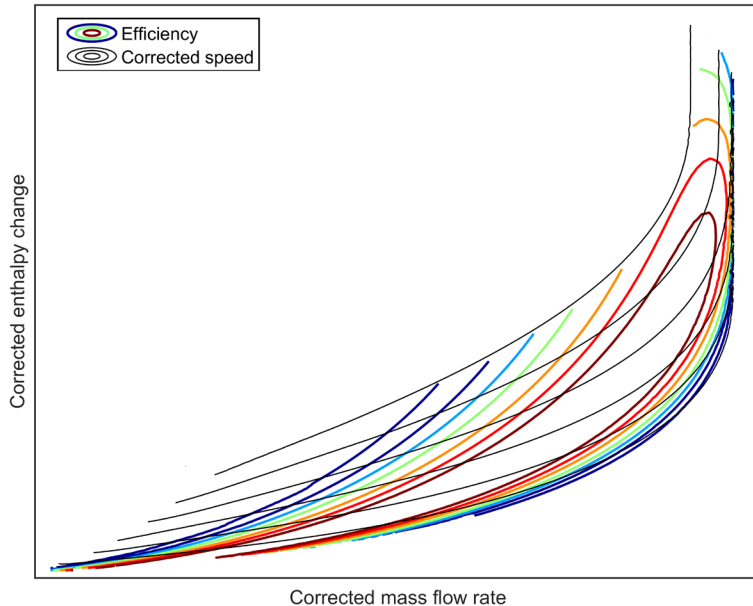
Standard approach bakes in ideal gas assumptions

Real gas (and dense-ish) fluid effects are more subtle. See, for example:

Pham, H. S. *et al.*, 2016, International Journal of Heat and Fluid Flow, **61**, pp. 379–394.

Variable inlet guide vanes add another dimension to maps

Turbine performance modeling – maps



Given inlet conditions and speed, can output pressure ratio and efficiency

Standard approach bakes in ideal gas assumptions

Real gas fluid effects are more subtle. See, for example, BNI's approach documented in Appendix B of:

Gavagnin, G., *et al.*, 2018, Applied Energy, **231**, pp. 660–676,
url=<https://linkinghub.elsevier.com/retrieve/pii/S030626191831451X>

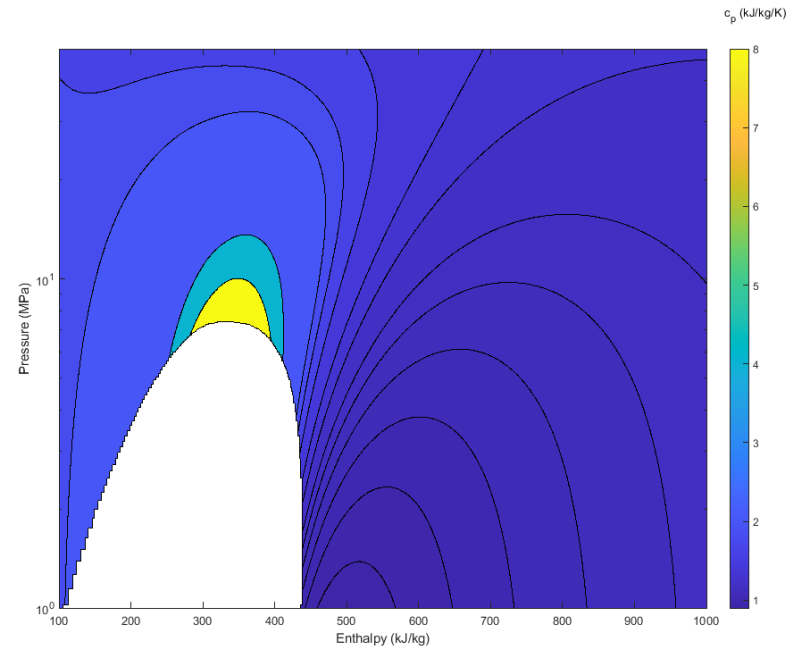
Variable inlet guide vanes add another dimension to maps

Heat exchangers

- 3 major categories:
 - Recuperators: Internal heat transfer (CO_2 to CO_2)
 - External heat addition: X to CO_2
 - External heat rejection: CO_2 to ambient (air or water)
- Common types for CO_2 :
 - PCHE/DBHE
 - Multi-bank finned tube
 - Shell & tube

Heat exchanger component models

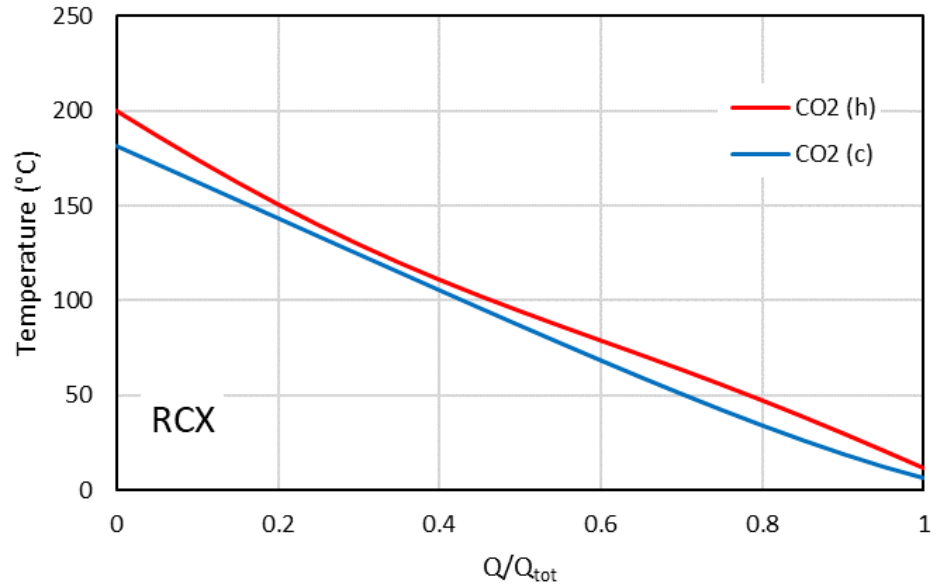
- Traditional approaches:
- Effectiveness/NTU
- UA LMTD
 - Both only work under constant c_p assumption
 - Bad assumption for CO_2 most of the time



Heat exchanger design point modeling - basic concepts

TQ plot example:

- Slope of curve is proportional to $(\dot{m}c_p)^{-1}$
- Ideal fluid with constant c_p , curves would be straight lines
- Real fluids have curves, and if the streams cross...



Heat exchanger design point modeling – more basics

- Heat transfer can be modeled as:

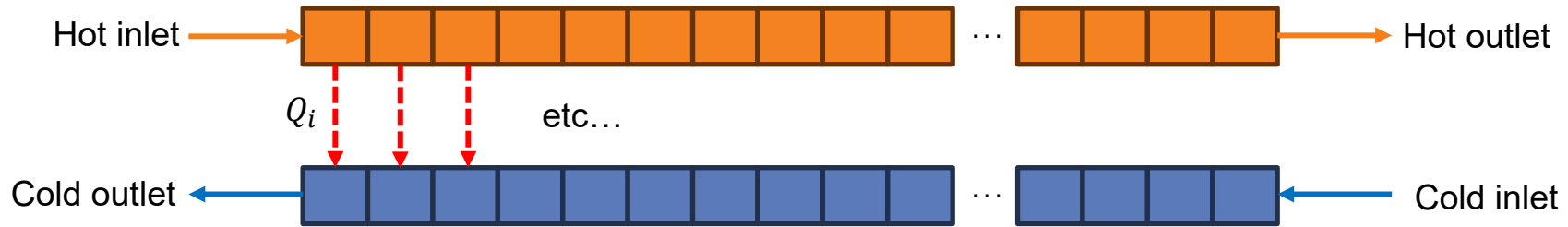
$$Q_h = -Q_c = \frac{\Delta T}{R} = UA \Delta T,$$

where R is a thermal resistance term that includes heat transfer area

and UA is the “conductance” of the heat exchanger

Heat exchanger design point modeling – one way

- Divide (discretize) heat exchanger into I segments



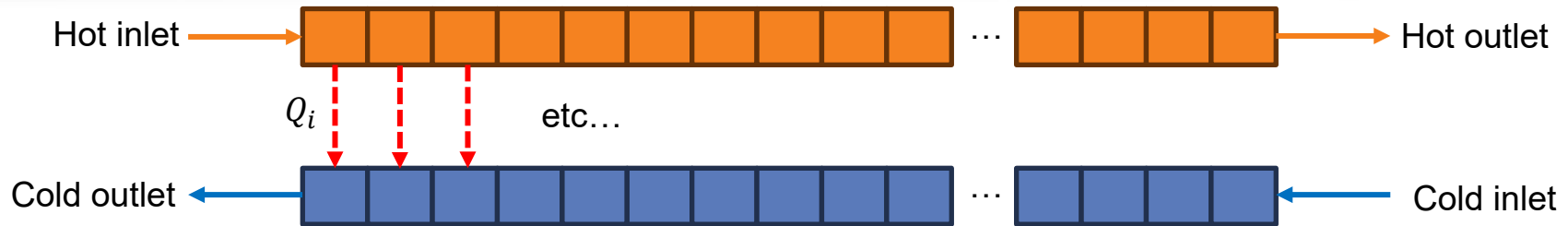
- By making I large enough, c_p of the fluids are reasonably constant in each interval, so we can write

$$Q = \sum_{i=1}^I dQ_i = \sum_{i=1}^I UA_i \Delta T_i$$

Heat exchanger design point modeling – Design mode

- Option 1: Specify a UA target
 - Given a set of inlet conditions (p, T, \dot{m}) , assume a set of outlet conditions such that $Q_h = -Q_c$
 - Calculate $Q_{total} = \dot{m}\Delta h$
 - Divide both sides into I segments of equal Q_i
 - Calculate $T_i = T(p, h_i)$
 - From preceding slide, $UA = \sum UA_i = \sum \frac{dQ_i}{\Delta T_i}$
 - Iterate on outlet conditions until $UA = \text{target value}$
- Other options include setting an effectiveness target or minimum temperature difference – iterative processes are similar
- Specified dP – check with suppliers to find out what is reasonable

Heat exchanger design point modeling continued



- Concept only applies to counterflow geometry
 - DBHEs are close to pure counterflow, but not exactly
- Cross-flow heat exchangers are common in air-to-CO₂ applications
 - If number of passes is > 3 or 4, counterflow isn't a bad approximation
 - More complex discretized solutions are possible, but might not be worth the effort – consider an effectiveness limit based on NTU

Heat exchanger modeling – performance

- Similar to design-point specified-UA technique
- Correct UA to off-design conditions

$$R = R_{conv,h} + R_{cond} + R_{conv,c}$$

$$R_{conv,h} = (h_{conv,h} A_{h,h})^{-1}$$

...etc

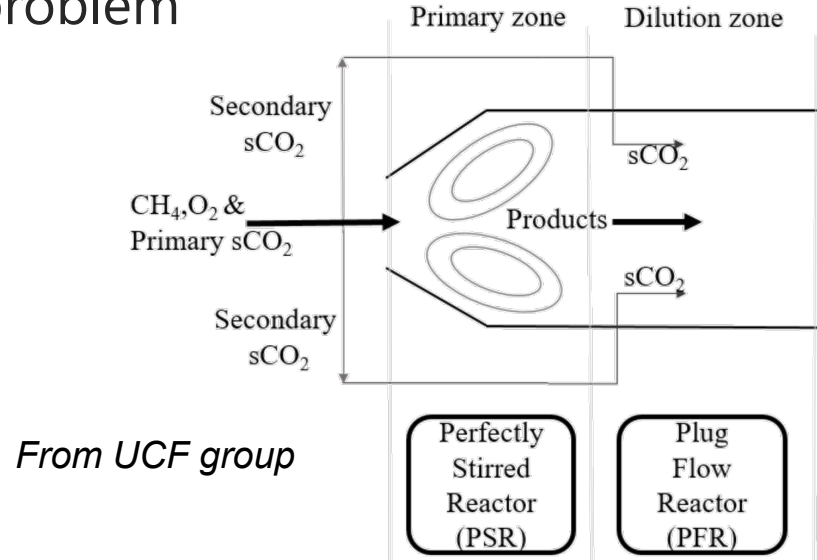
using your favorite heat transfer correlation(s) ($Nu = hd/k = f(Re, Pr, \dots)$), ratioed to design point

- Correct dP using a similar approach:

$$dP = \frac{f(Re)}{d} \frac{\rho}{2} U^2 L$$

Oxy-fuel combustion in CO₂

- Standard equilibrium solvers (e.g. Chemkin, ASPEN) will manage $T(h_{in}, X_f, X_o)$ problem
- Kinetics simulations – wide-open problem!



Other modeling tips

- Heat losses can be significant, especially in small systems – consider including in modeling
- Piping pressure drops are also important, model similarly to heat exchanger dP
- Control valves are frequently necessary to adjust flow splits and have non-zero dP even when full open
- Secondary / auxiliary loads need accounting
 - Cooling fans, pumps, etc.
 - Seal gas conditioning systems
 - Lube oil cooling
 - Generator, gearbox, VFD, switchgear losses

Fluid properties

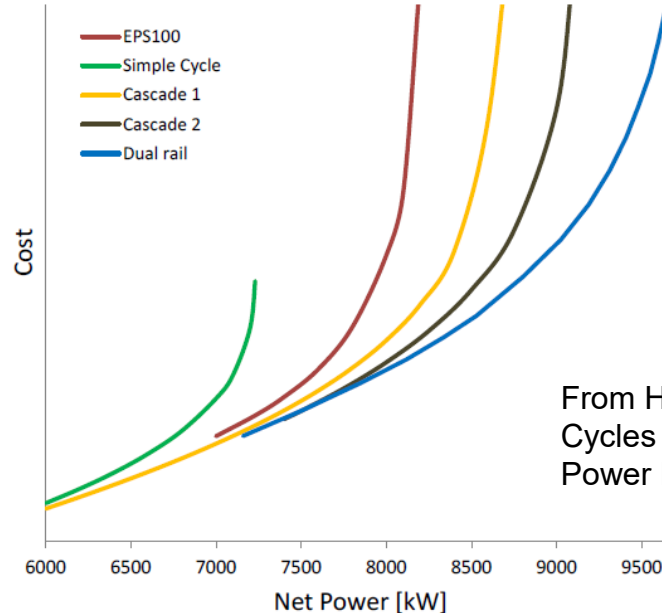
- Span & Wagner EOS for CO₂ is industry standard
- New EOS has been created (Harvey and Lemmon, 2022 sCO₂ Symposium) – release date TBD (but not imminent)
- REFPROP, CoolProp both use S&W
 - Generally good for pure CO₂
 - Mixture properties less certain
 - Execution speed can be problematic
 - 2-D table lookups a common approach
 - Interpolation behavior near saturation line can be a problem
 - $h_{\text{lookup}} = h(T_{\text{spec}}, P), T_{\text{lookup}} = T(h_{\text{lookup}}, P), \dots T_{\text{lookup}} - T_{\text{spec}} \neq 0!$
 - Not necessarily the end of the world, but can be a problem if you expected that behavior

Cost modeling

- Core function of practical modeling – cost/performance trades

- Key cost variables:

Cycle complexity
Heat exchanger sizing



From Held, 2015, "Supercritical CO₂ Cycles for Gas Turbine Combined Cycle Power Plants," *Power Gen International*.

Cost modeling (continued)

- Typical cost models:

$$C = A + B \cdot SP^n$$

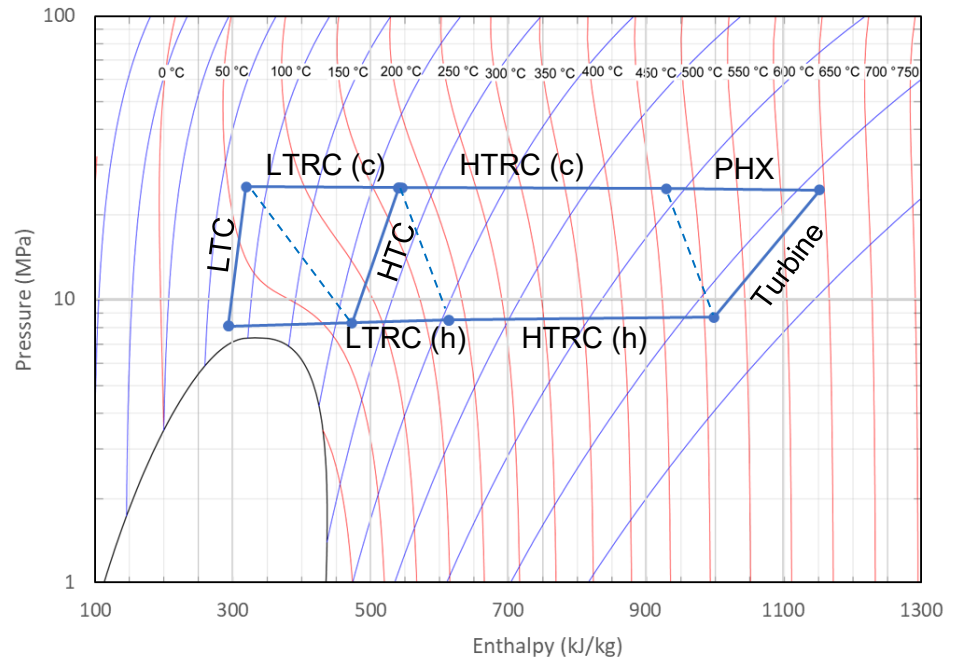
where “ SP ” is a scaling parameter (e.g., UA for heat exchangers, power output for turbines, etc.), A , B and n are fit parameters

- Weiland paper is an excellent source for fit parameters – recognizing that 2024 prices are 1.3 to 1.5X vs 2019

Weiland, Lance and Pidaparti, “sCO₂ Power Cycle Component Cost Correlations from DOE Data Spanning Multiple Scales and Applications,” *ASME Turbo Expo 2019*, Paper GT2019-90493

Modeling tools and techniques

- Hand draw on a PH diagram – great way to get into the ballpark



Modeling tools

- Spreadsheet models
 - Good way to get started, teaches you how to set up a problem, what's missing
 - Anything more complicated than an unrecuperated cycle will require iteration
 - Potentially error-prone
- MATLAB, Python
 - Largely still "roll-your-own" approach
 - Much larger selection of optimization methods
 - Also error-prone

State	Outlet	Inlet	h (kJ/kg)	P (MPa)	T (°C)	s (kJ/kg·K)	w (kg/s)	Q/W (kW)
1	ACC	LTC	293.60	8.05	31.73	1.303	599.28	-107687
2	LTC	LTRc	319.78	24.99	62.15	1.312	599.28	15690
31	LTRc	Mix	546.07	24.79	175.36	1.900	599.28	135611
32	HTC	Mix	540.83	24.79	172.05	1.888	363.18	
33	Mix	HTRc	544.09	24.79	174.11	1.896	962.46	
34	HTRc	PHX	929.87	24.59	468.17	2.566	962.46	371299
4	PHX	HPT	1153.06	24.34	645.93	2.838	962.46	214809
5	HPT	HTRh	999.45	8.65	512.82	2.858	962.46	-147843
54	HTRh	LTRh	613.67	8.45	178.86	2.225	962.46	-371299
6	LTRh	ACC	473.29	8.25	70.13	1.871	962.46	-135111
32	Compr outlet (check		540.83	24.79	172.05	1.888	363.18	24530
	Wt	-147843	kW		Aux loads & losses			
	Whtr	24530	kW		Generator	-1478		
	Wlrc	15690	kW		Motor/VF	-402		
	Wnet	100643	kW		Misc	-50		
	Qh	214809	kW		Heat source	-512		
	Qc	-107687	kW		Coolant	-4538		
	Eta	46.85%			Total	-6981		
	UAltr	21636	0.976352					
	UAhtr	15395	0.985902					
	UAacc	18907	0.945277					
	UAphx	1648	0.575364					

Modeling tools - Constraints

- Non-linear optimizers need boundaries – and a good initial guess

Variables	x	LB	UB	x0
P1	8.05	7	12	8
P2	24.99	10	25	25
T1	31.73	28	60	30
T31	175.36	100	400	170
T34	468.17	200	600	450
T4	645.93	600	650	640
wltc	599.28	5	800	600
whtc	363.18	0.1	400	350

Constraints		LB	UB
LTC margin	1.052	0.3	
UALTR	21636		40000
UAHTR	15395		30000
UAACC	18907		20000
UAPHX	1648		10000
Wnet	100643	100000	100001
HX cost	52,970,721		54,000,000

Modeling tools – not an exhaustive list!

- Commercial codes
 - ASPEN, HYSYS, Ebsilon, GateCycle, IPSEPro, AxSTREAM, CYCAL, NPSS, Flownex, Modelon
- Open-source codes
 - OpenMDAO/PyCycle, T-MATS, others?

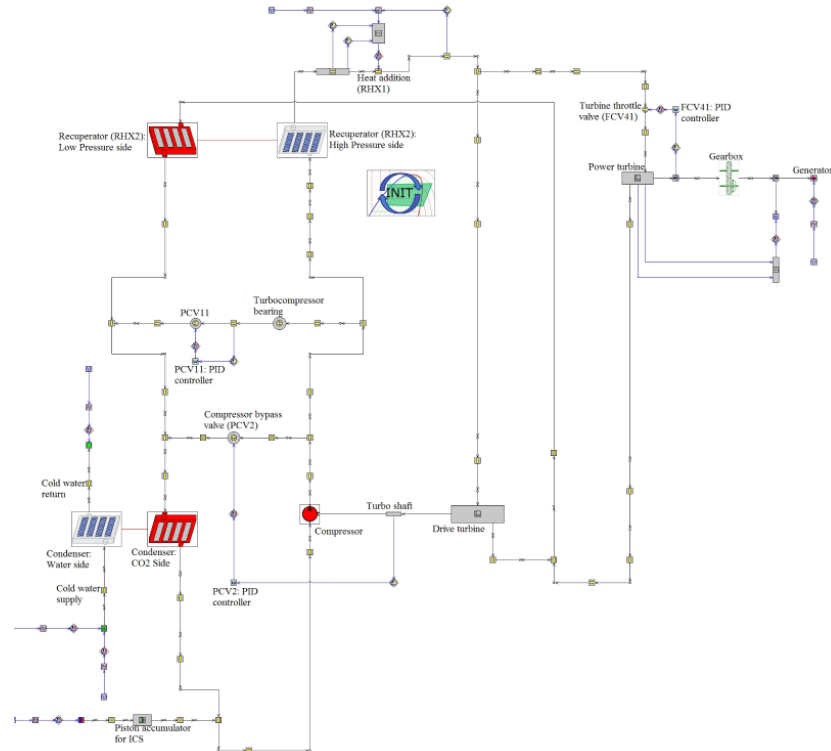
Transient modeling

- Simulation purposes:
 - System responses to changes in power demand, heat supply, heat sink temperature
 - Control system design and optimization
 - Startup/normal shutdown
 - Event simulation – e-stops, PRV releases, pipe ruptures
 - Define transient BCs for components, transient stress analysis
- Significantly more challenging numerically, computationally
- Requires at least a rudimentary control system layout
- Requires component off-design models
- Steady-state models + transient terms
 - Thermal inertia
 - Mechanical inertia
 - Volume dynamics (fluid inertia)

Transient model example

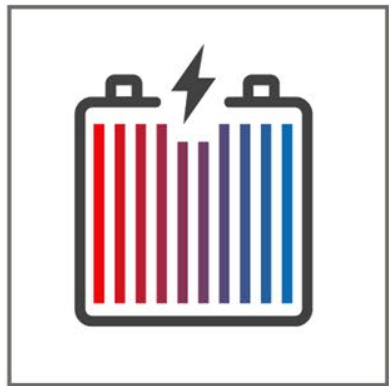
- Model construction similar to steady-state model
- Setting up BCs and ICs crucial to finding valid solution

From Avadhanula and Held, "Transient Modeling of a Supercritical CO₂ Power Cycle and Comparison with Test Data," *ASME Turbo Expo 2017*, GT2017-63279



Transient modeling tools – not an exhaustive list!

- Commercial codes
 - Aspen, NPSS, Flownex, Modelon, GT-SUITE, AME-Sim, TRNSYS, MATLAB-Simulink, Dymola
- Open-source codes
 - Modelica (language, not a program)



Q&A