8th sCO₂ Symposium

San Antonio, TX February 26-29, 2024

Cycles Tutorial

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Motivation for CO₂ as a Working Fluid





High Efficiency

Smaller Turbomachinery

Renewed interest due to enabling advances in:

- Materials (USC, AUSC programs)
- Dry Gas Seals (more experience in CO₂ and LNG compressors)
- Compact Heat Exchangers

Work on sCO2 predates Dostal



Feher 1967

1. Feher, E. G., "The Supercritical Thermodynamic Power Cycle," Douglas Paper No. 4348, presented to the Intersociety Energy Conversion Engineering Conference, Miami Beach, Florida 13-17 Aug. 1967.

AFAPL-TR-68-100

INVESTIGATION OF SUPERCRITICAL (FEHER) CYCLE

E. G. Feher et al.

Astropower Laboratory, Missile & Space Systems Division A Division of McDonnell Douglas Corporation

TECHNICAL REPORT AFAPL-TR-68-100

October 1968



Angelino 1968

Carbon Dioxide Condensation Cycles For Power Production G. ANGELINO Lecturer of Special Power Plants, Politecnico, Milan, Italy The thermodynamic performance of several condensation cycles employing carbon

dioxide as working medium is analysed and discussed. A balanced distribution of hermodynamic losses between mechanical components and heat exchangers attained through a compression performed partially in the light and partially in the gas phase yields cycle efficiencies which are among the highest achievable in present-day energy systems. At turbine inlet temperatures higher than 650 deg C single heating CO2 cycles exhibit a better efficiency than reheat steam cycles. This may prove of particular interest in connection with high temperature nuclear heat sources. However, the requirement of low temperature cooling water for a good cycle arrangement represents a geographical limitation to the widespread application of CO₂ condensation cycles.

Introduction

bine inlet temperatures. The cycle arrangement retains almost the same simplicity as the gas turbine configuration. However, ARGE capacity steam power stations represent the due to the low critical temperature of carbon dioxide, condensing most efficient tool for the conversion of heat into mechanical evcles are obtainable only in countries where cooling water at temperatures not higher than 12-15 deg C is available the year

energy. After a rapid improvement of cycle configuration and equipment during the last two decades, steam plants reveal at round. present some thermodynamic and technological limitations for units of growing output. Stations employing the closed-cycle gas turbine are character-ized by a simpler arrangement of the components and by the point of view (full advantage can be taken of the low tempera-Stations employing the closed-cycle gas turbine are characterability to take full advantage of increasing maximum temperatures. However, their efficiency, even for the highest practical danger of solidification of the working fluid during shutdown temperatures, is considerably lower than that of current steam periods). stations. Condensing or partially condensing cycles employing carbon dioxide as a working medium allow the achievement of efficiencies tion of earbon dioxide condensing cycles. Hydraulic works similar to that of steam cycles, or even better for the highest tur-Contributed by the Gas Turbine Division and presented at the Gas Turbine Conference, Washington, D. C., March 17–21, 1965, of Tura Aurancus Noczerry or MicraAurach Econstruens, Manu-script received at ASME Headquarters, December 28, 1967. Paper No. 68-CT-28.

Deep water temperature of the largest European or North which may be a hindrance to further developments. These limitations can be summarized as follows: (a) Cycle economy is not very sensitive to the rise of the tribine inlet temperature (while the temperature of the Mediterramean, at the depth beyond about 600 deg C; (b) cycle complexity increases with the of 500 m, has the constant value of about 13 deg C). Along the water heating lines and additional low pressure turbine soctions year. In these regions the use of carbon dioxide as working

> ture of the cold source) and for technological reasons (there is no The requirement of abundant, low temperature water for larger than required by steam stations could be necessary; however, their influence on the overall station economy should not

be prominent **Cycle Configurations** For carbon dioxide cycles, as for steam, a variety of cycle

Journal of Engineering for Power

-Nomenclature

Copyright © 1968 by ASME

Dostal 2004



High Efficiency



sCO2 Application Space





Basic Components in a Simple Recuprated Cycle





Compress Expand Recuperate



What's Special about CO₂?





T-s Diagram for CO2 with typical high temperature recompression cycle

Note ambient temperature is near the critical point

Pink lines are constant enthalpy – horizontal indicates h=Cp*T is valid

What's Special about CO₂?





Close up of low T region

Constant enthalpy lines far from horizontal

Quiz



★ Statepoint 1 is at 82.4 bara and 34.2 C
★ Statepoint 2 is at 75.0 bara and 32.0 C

Which has a higher enthalpy?

SwRI

Quiz

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★ Statepoint 2 is at 75.0 bara and 32.0 C

Which has a higher enthalpy?



Southwest Research Institute

Common CO₂ Equations of State





Important to use Refprop to ensure accuracy of EOS

Carnot vs Lorenz





Southwest Research Institute



Applications and Architetures

SOUTHWEST RESEARCH INSTITUTE

High Temperature Cycles

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sCO₂ Recompression Cycle





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High Temperature Cycles – Thermodynamic Benefit



150 C increase in average heat addition temperature

ightarrow 6.8 pts in Carnot efficiency



High Temperature Cycles – Flow Differences





Specific Heat Input $CO_2 = 307 \text{ kJ/kg}$ $H_2O = 3040 \text{ kJ/kg}$

 CO_2 mass circulation ~10X H₂O



CO₂ Requires Larger Pipes for Hot Flows

 CO_2 Turbine Exit Vol Flow ~0.03X H₂O \rightarrow CO₂ Turbines much smaller

Waste Heat Recovery

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Waste Heat Recovery – Thermodynamic Benefit



Heat Transferred

Fundamentally different benefit vs High Temperature cycles

Cascaded CO₂ Bottoming Cycle



Cascaded cycle uses two sCO₂ loops to maximize performance

CO₂ circulates in two closed loop cycles – only small make-up for shaft seal leakages

Small equipment size enables BC to approach aeroderivative transient performance

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Impact of Ambient Temperature



GE data : P. Huck, M. Lehar, "Performance comparison of a supercritical CO2 versus steam bottoming cycles for aeroderivative gas turbines at various ambient temperature," ChemIndix, Nov 2016, Manama, Bahrain

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Condensing Cycles



- Transcritical cycle
- Utilizes partial compression, condensation, and pumping to minimize compression work
- Must balance refrigeration / cooling requirements against compression requirements
- Can achieve efficiencies close to recompression cycle





Allam (Direct Oxy-Fuel) Cycles

- Direct fire oxy-fuel combustion changes the cycle to a semiopen cycle
- Mass balance issues
- CO2 + combustion products
- Clean up and water removal Removal







sCO₂ Heat Pumps for Industrial Heat and ETES





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 $N_{var} = N_{DOF}$, you are solving for a single unique solution
 - If $N_{var} > N_{DOF}$, 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



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Component operating conditions affect how you model them



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

* Simple compressible substance, with known EOS

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



Corrected mass flow rate

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=<u>https://linkinghub.elsevier.com/retrieve/pii</u> /S030626191831451X

Variable inlet guide vanes add another dimension to maps

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Heat exchangers

- 3 major categories:
 - Recuperators: Internal heat transfer (CO₂ to CO₂)
 - External heat addition: X to CO₂
 - External heat rejection: CO₂ to ambient (air or water)
- Common types for CO₂:
 - 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 CO₂ 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=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
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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, ...)), 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
 Primary zone Dilution zone
- 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
 - $h_{lookup} = h(T_{spec'}P), T_{lookup} = T(h_{lookup'}P), ... T_{lookup} T_{spec} \neq 0!$
 - 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



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	Р	Т	s	w	Q/W
			(kJ/kg)	(MPa)	(°C)	(kJ/kg·K)	(kg/s)	(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			
	Whtc	24530	kW		Generator	-1478		
	Wltc	15690	kW		Motor/VF	-402		
	Wnet	100643	kW		Misc	-50		
	Qh	214809	kW		Heat sour	-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				FCH	()(÷ł

Modeling tools - Constraints

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

х	LB	UB	x0
8.05	7	12	8
24.99	10	25	25
31.73	28	60	30
175.36	100	400	170
468.17	200	600	450
645.93	600	650	640
599.28	5	800	600
363.18	0.1	400	350
	LB	UB	
1.052	0.3		
21636		40000	
15395		30000	
18907		20000	
1648		10000	
100643	100000	100001	
52,970,721		54,000,000	
	x 8.05 24.99 31.73 175.36 468.17 645.93 599.28 363.18 1.052 21636 15395 18907 1648 100643 52,970,721	x LB 8.05 7 24.99 10 31.73 28 175.36 100 468.17 200 645.93 600 599.28 5 363.18 0.1 LB 1 1.052 0.3 2.1636 1 1.5395 1 1.8907 1 1648 100000 52,970,721 1	NLBUB8.057128.0571224.99102531.732860175.36100400468.17200600645.93600650599.28600650363.180.14001005100400010050.34000110520.3300001539510030000164810000100011006431000054,000,000



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

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- 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)

