R&D activities on sCO_2 in Europe

Back to basics: status of the sCO_2 fundamental research

9th episode – 30 September 2025

Webinar speakers

Session moderator

- David Sánchez (University of Seville)

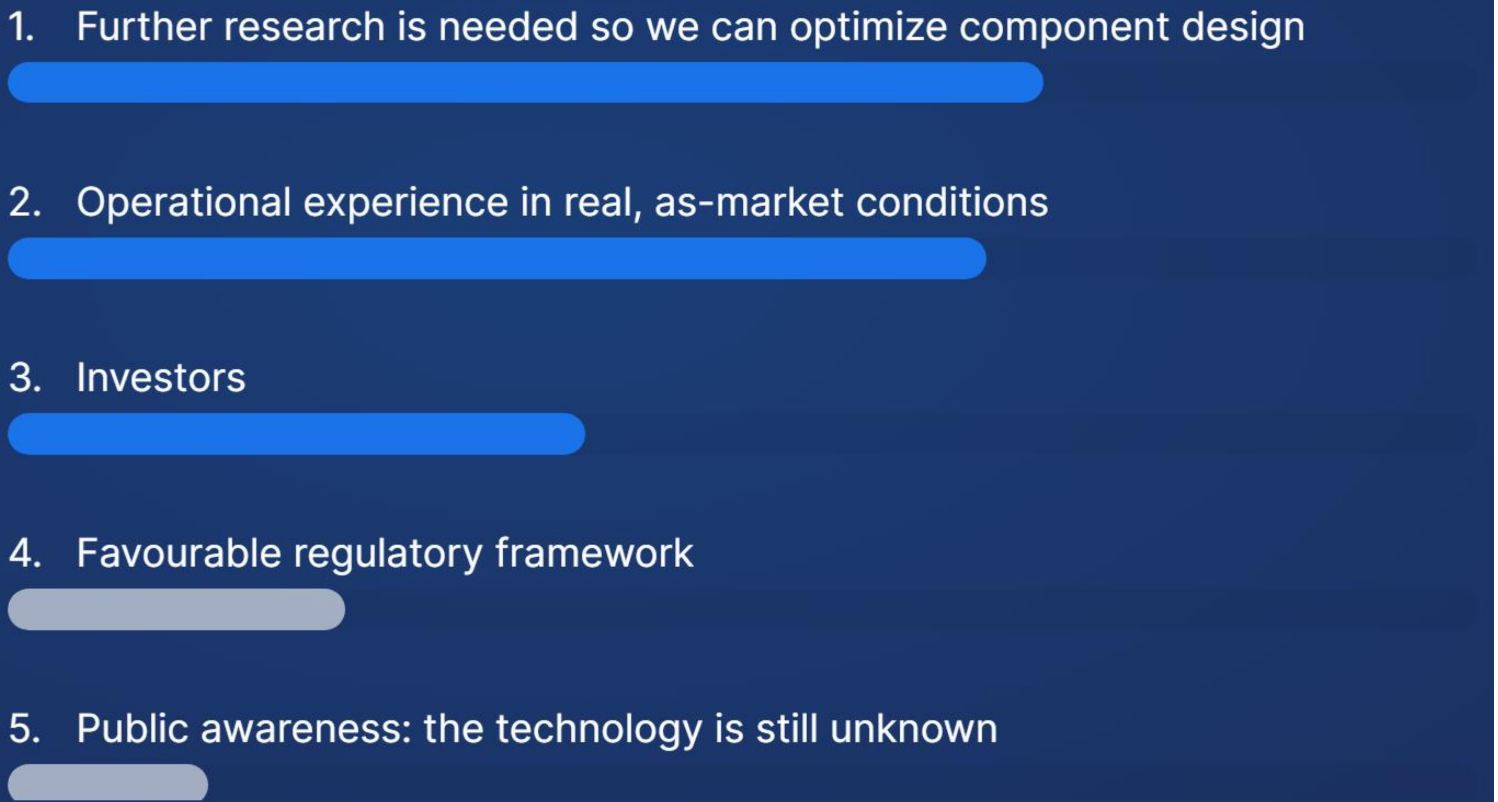
Speakers

- Alessandro Romei (Politecnico di Milano)

- Rene Pecnik (TU Delft)

- Henry Saari (Carleton University)

What is the main challenge preventing commercial sCO2 projects from being developed?

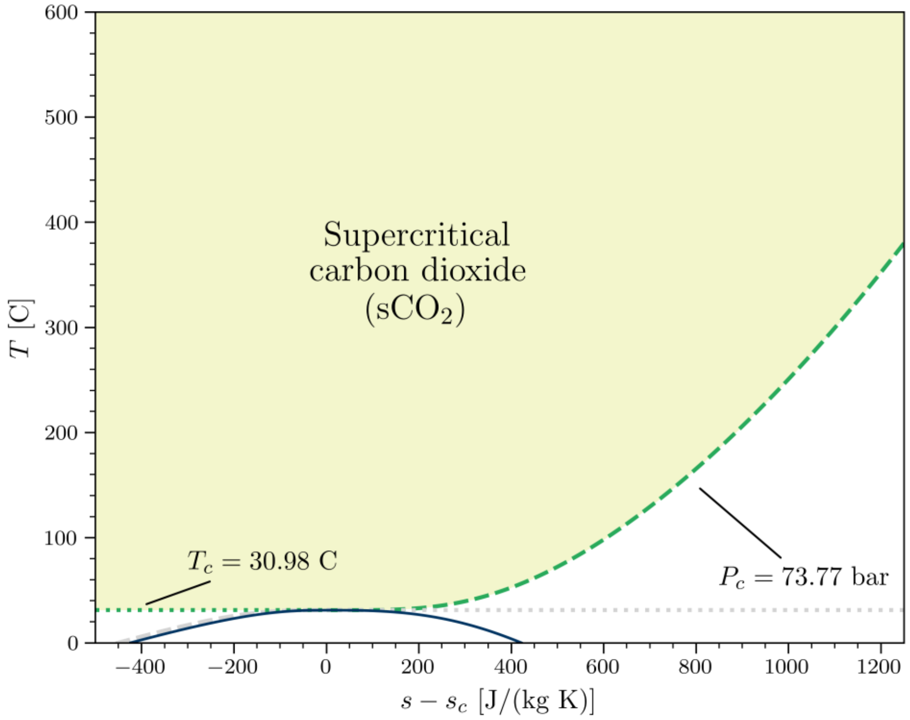


ETN Global

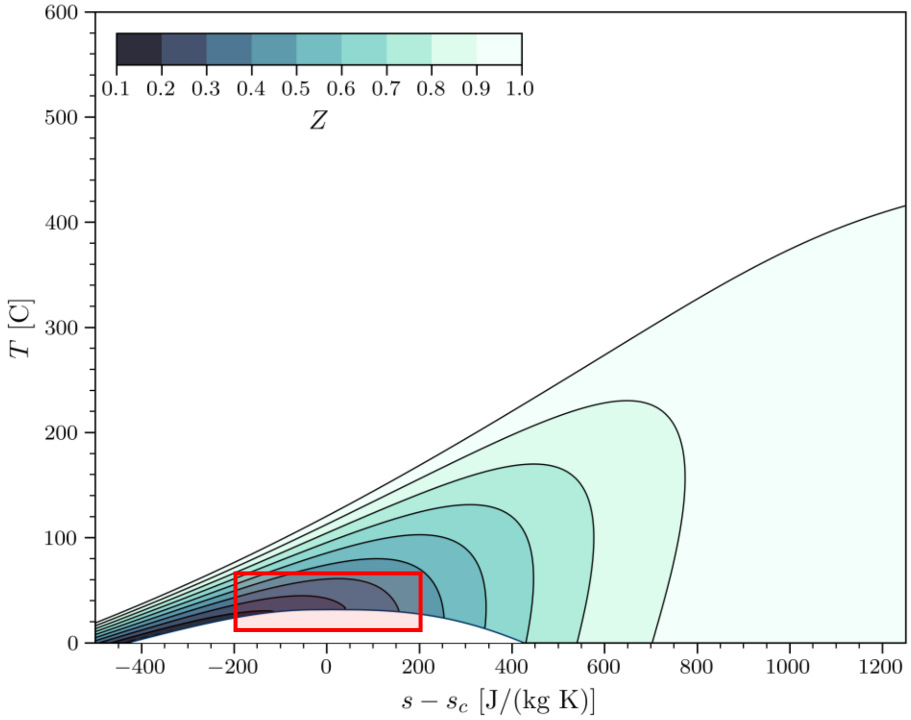
Back to basics: Status of the sCO_2 fundamental research – Fluid Dynamics

Alessandro Romei, Politecnico di Milano

Supercritical carbon dioxide (sCO_2)



Supercritical carbon dioxide (sCO_2)



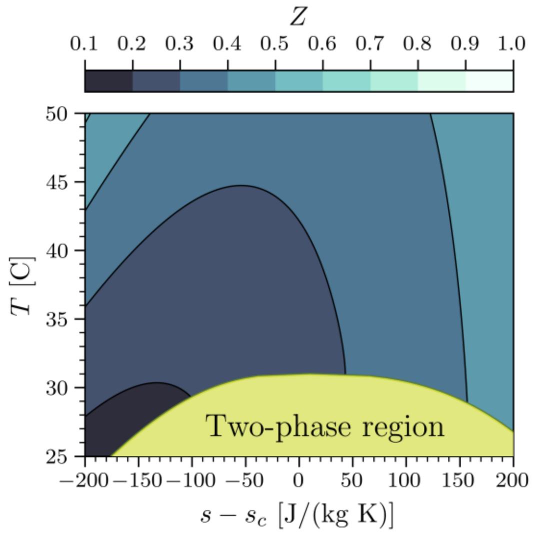
$$Z = \frac{v}{v_{ideal}}$$ Compressibility factor

$Z \ll 1$ Near-critical region

Departure from ideal-gas modelling

Applications: sCO_2 compressors, ejectors and turbines for heat pumps

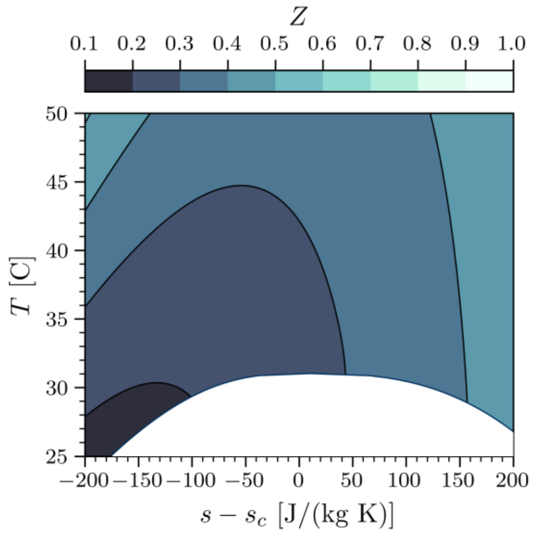
Challanges in near-critical region



Non-ideal thermodynamics

Occurrence of two-phase flows

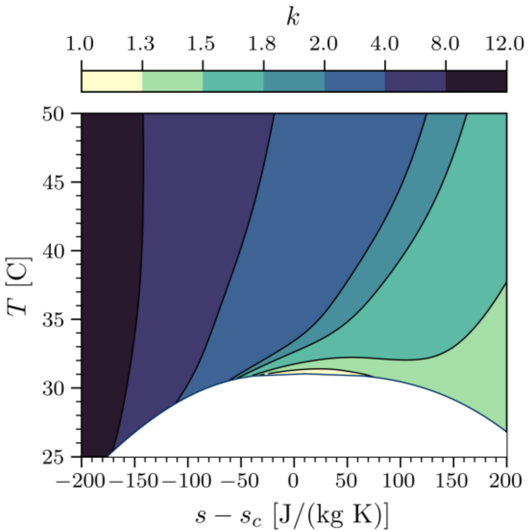
Compressibility factor



Z quantifies the **volumetric deviations** from the ideal gas law.

"*Static*" parameter: <u>its role on fluid dynamics is not directly interpretable.</u>

Generalized isentropic coefficient



Generalized isentropic coefficient
(also known as pressure-volume isentropic coefficient)

$$k \stackrel{\text{def}}{=} -\frac{v}{P}\left(\frac{\partial P}{\partial v}\right)_s = -\frac{v}{P}\frac{c_p}{c_v}\left(\frac{\partial P}{\partial v}\right)_T$$

$$k \to \frac{c_p}{c_v} = \gamma$$ with ideal-gas model

Generalized isentropic coefficient

Isentropic flow of ideal gas:

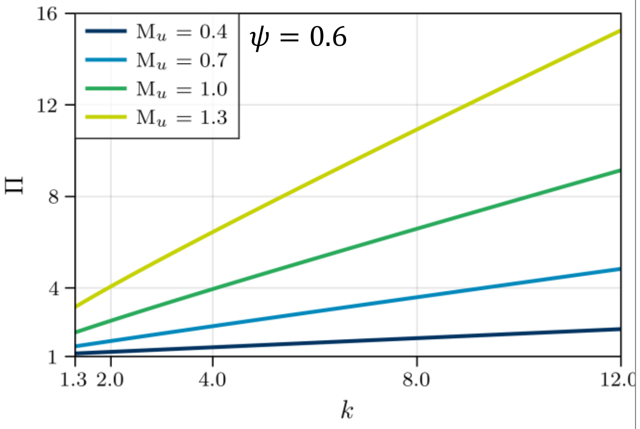
$$\Delta h = \frac{\gamma}{\gamma - 1} R T_1 \left(\Pi^{\frac{\gamma-1}{\gamma}} - 1 \right)$$

Isentropic flow of general fluid:

$$\Delta h \approx \frac{k}{k - 1} Z_1 R T_1 \left(\Pi^{\frac{k-1}{k}} - 1 \right)$$

Dimensionless form for a machine:

$$\psi = \frac{\Delta h}{u^2} = \frac{1}{M_u^2} \frac{1}{k - 1} \left(\Pi^{\frac{k-1}{k}} - 1 \right)$$

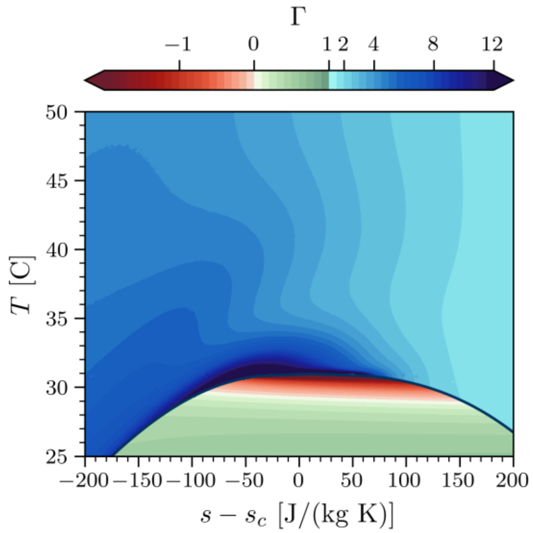


Vapor-like

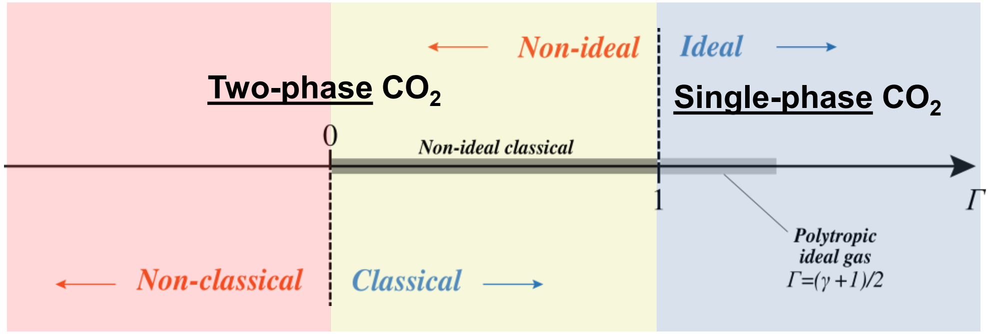
Liquid-like

Romei & Persico (2021), "On sCO_2 compressor performance maps at variable intake thermodynamic conditions", ASME Paper GT2021-60252

Fundamental derivative of gasdynamics



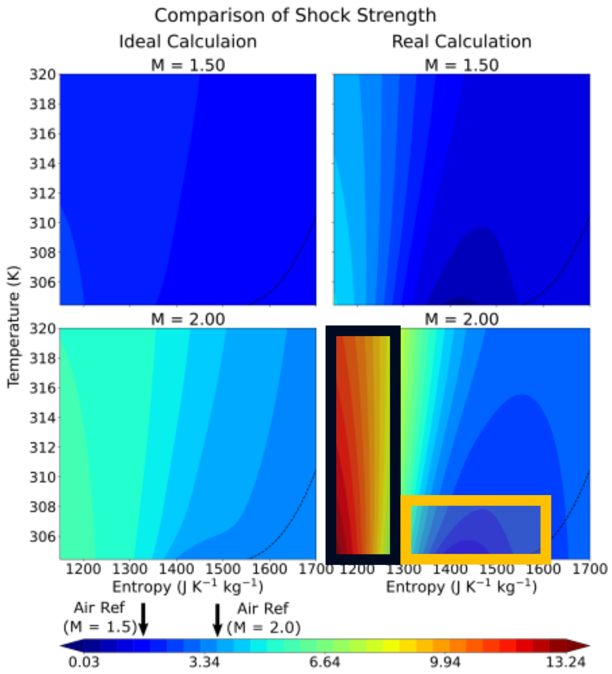
$$\Gamma = 1 + \frac{c}{v}\left(\frac{\partial c}{\partial P}\right)_s$$



- Rarefaction shocks

- Non-monotonic Mach number
- Mach number increase through oblique shocks

Implications on shocks



Symbolic regression automatically provides a **direct relationship** among shock strength, k and Γ

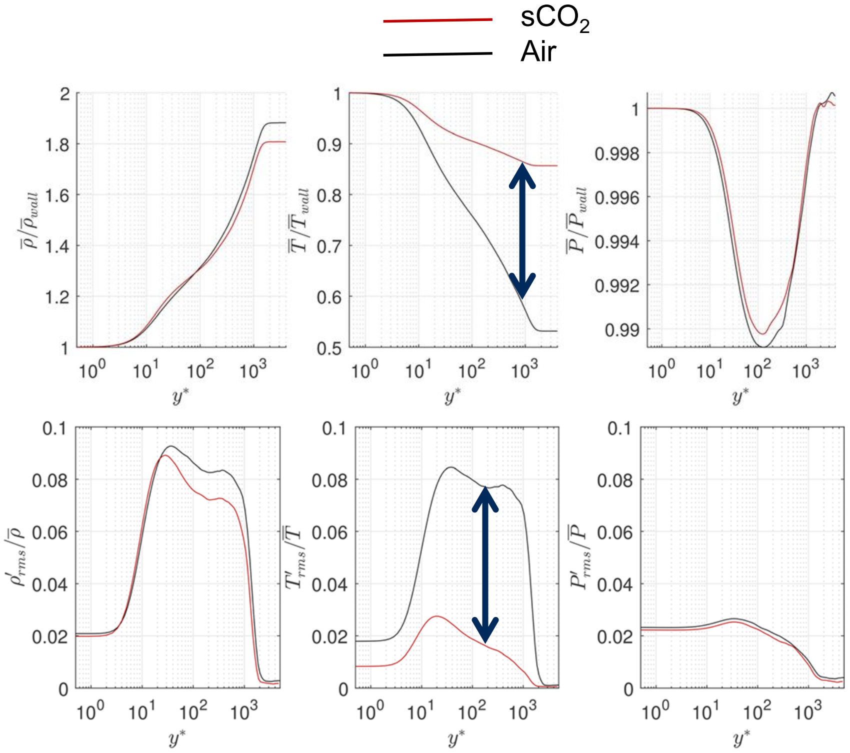
$$\text{Shock Strength} = \frac{k_1\, M_1^2(M_1^2 - 1)}{\Gamma_1 M_1 + M_1^2 - 1}$$

Liquid-like shocks stronger than ideal-gas shocks

Near-critical shocks weaker than ideal-gas shocks

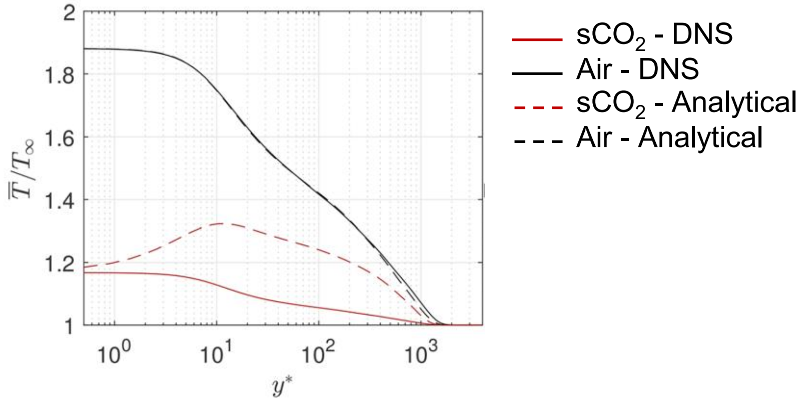
Wang et al. (2023), "Supercritical Carbon Dioxide Shock Behavior Near the Critical Point", J. Eng. Gas Turbines Power.

High-speed sCO_2 boundary layer



Small Eckert number, $E_c = \frac{u^2}{c_p T}$

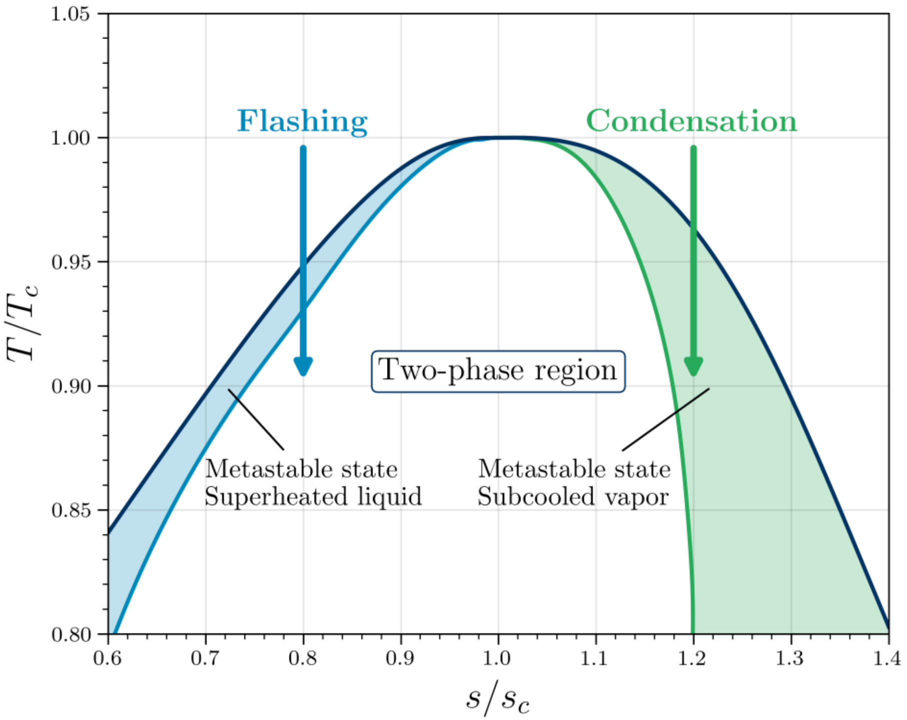
↳ reduced temperature variations



Warning: commercial CFD solvers may use temperature scaling methods for wall functions

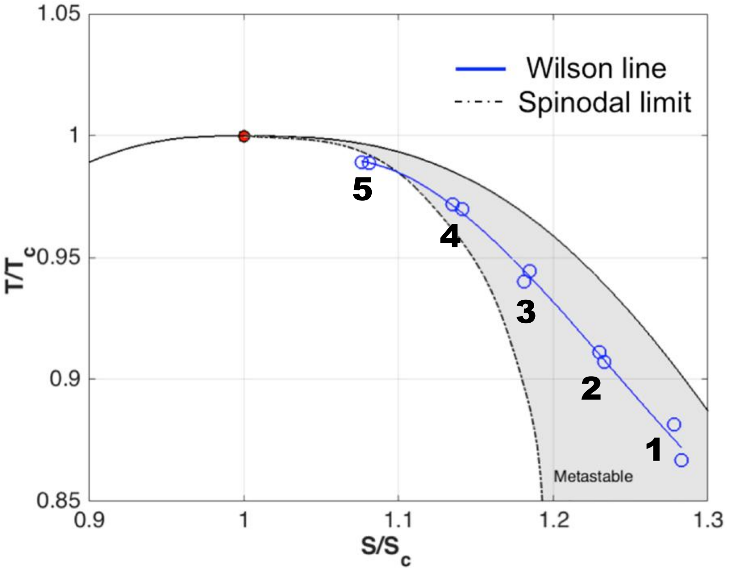
Wang (2025), "Direct numerical simulation of the supersonic turbulent boundary layer of supercritical carbon dioxide", Phys. Fluids.

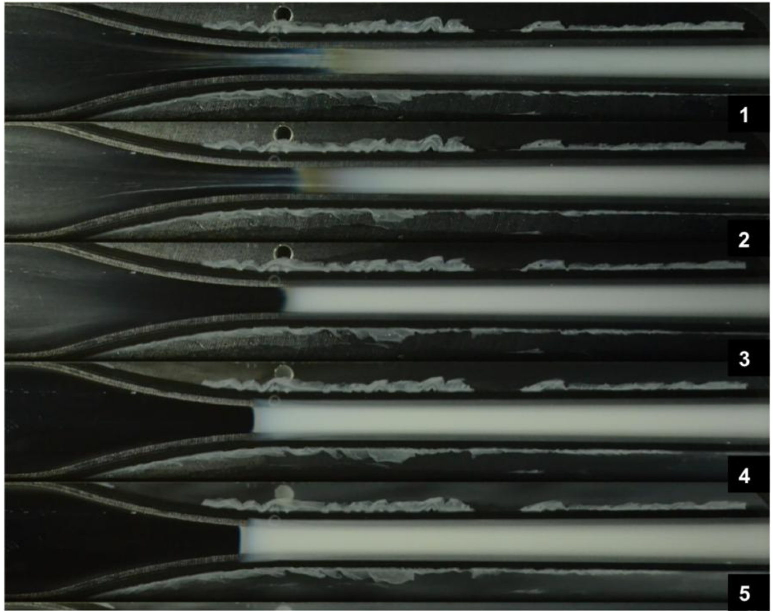
Two-phase flows



Metastable effects reduces near critical point

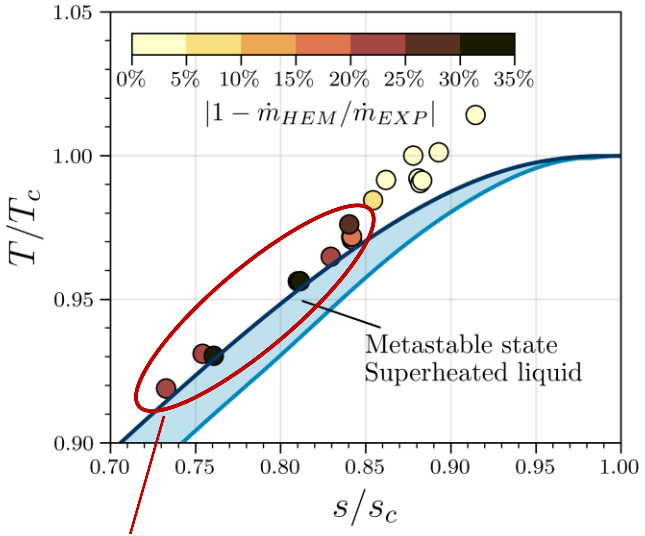
Equation of state extrapolation yields errors as large as 2%



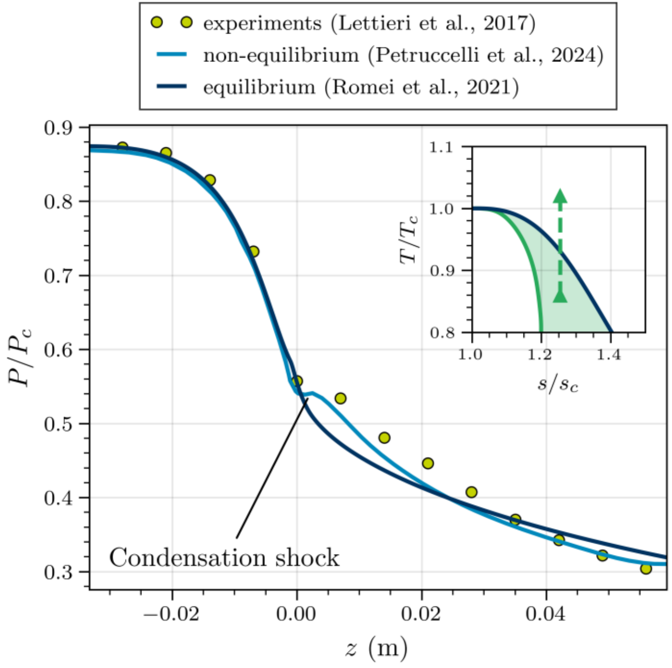


ri et al. (2018), "Characterization of Nonequilibrium Condensation of Supercritical Carbon Dioxide in a de Laval Nozzle “, J. Eng. Gas Turbines Power.

Limits of homogeneous equilibrium

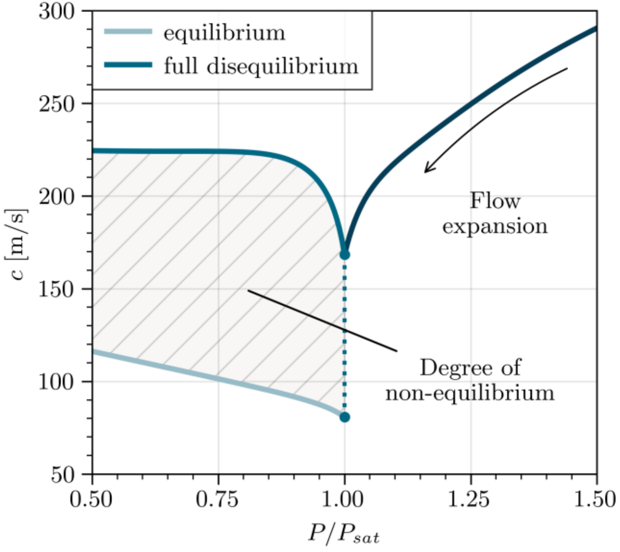


Deviations up to 35%
assuming thermodynamic equilibrium

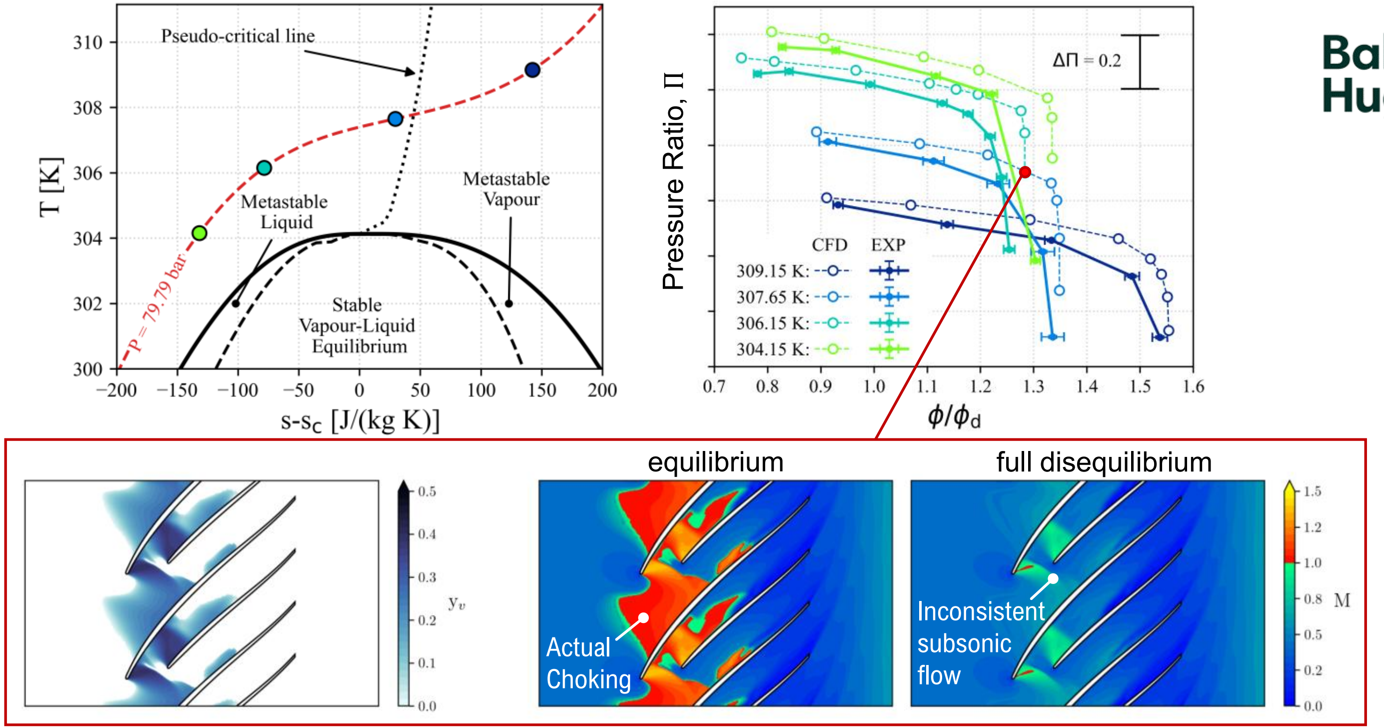


Palacz et al. (2017), "HEM and HRM accuracy comparison for the simulation of CO2 expansion in two-phase ejectors for supermarket refrigeration systems", Appl. Therm. Eng.
Romei et al. (2021), "Computational fluid-dynamic modelling of two-phase compressible flows of carbon dioxide in supercritical conditions", Appl. Therm. Eng.
Petruccelli et al. (2024), "A novel numerical approach for simulating low-pressure and high-pressure non-equilibrium condensation in real gases", Int. J. Multiph. Flow

«Two-phase» speed of sound



Experimental evidence on MW-scale compressor



Conclusion and research gaps

Fascinating fluid-dynamic problem

Multiple effects need to be considered (non-ideal thermodynamics, two-phase flows, unconventional shocks, non-equilibrium effects)

Further experiments are needed

Some effects (e.g., two-phase non-equilibrium) are studied with semi-empirical models derived from other fluids/operating conditions

Understanding the implications on sCO_2-based technologies

Quantify the impact of this peculiar fluid dynamics on machines, ejectors, heat exchangers

Status of the sCO_2 fundamental research – Fluid Dynamics

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Back to basics: Status of sCO_2 fundamental research – Heat transfer

Rene Pecnik, Delft University of Technology

Acknowledgements

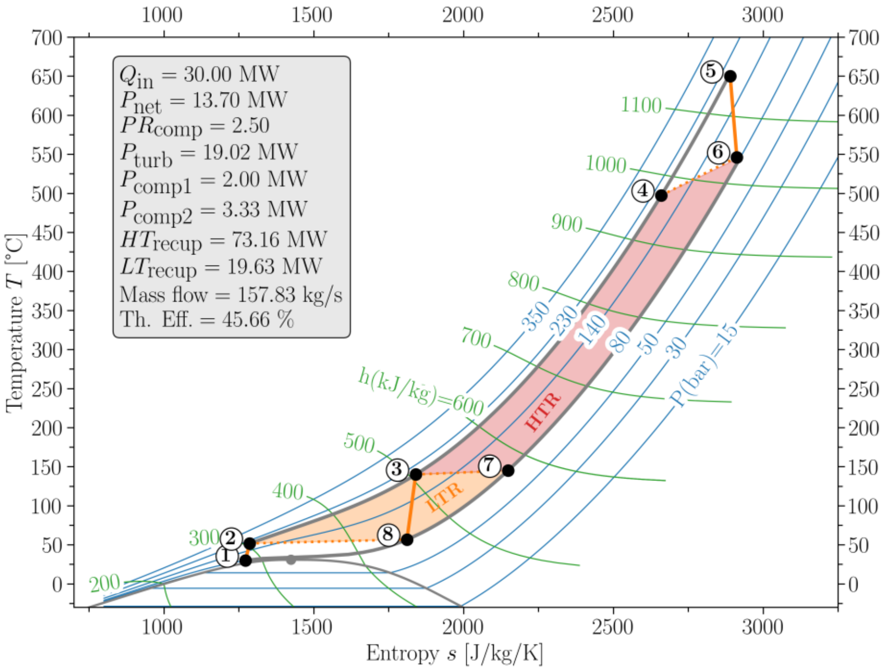
- **Funding**

CRITICAL
Grant agreement ID: 864660
(2020-present)

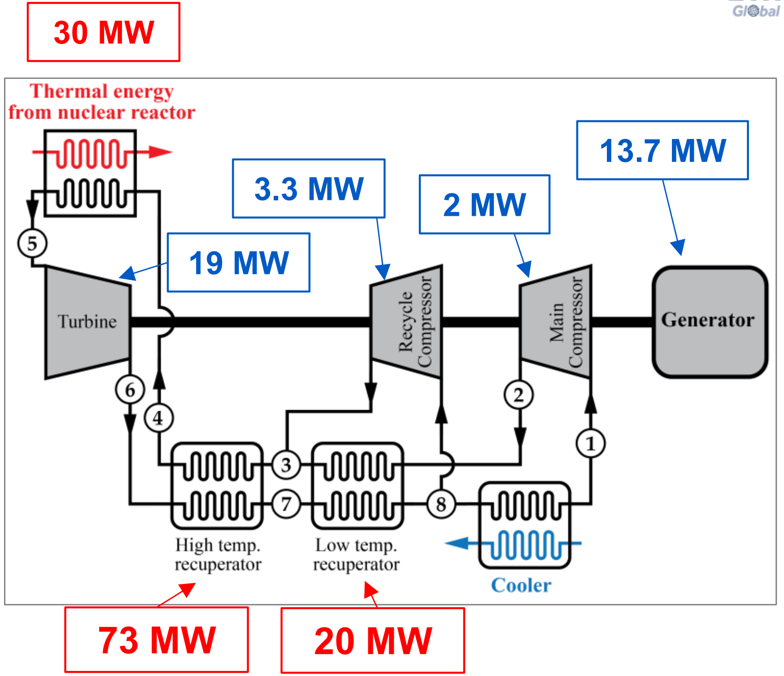
- **PhDs, Postdocs**
  - Asif Hasan, Marko Draskic, Pietro Boldini, Benjamin Bugeat

- **Collaborators**
  - Jurriaan Peeters (TUD), Pedro Costa (TUD)
  - Colleagues from Univ. Maryland, Sapienza U. Rome, ESSS Brazil, Ansys Inc.

Motivation – Heat Transfer



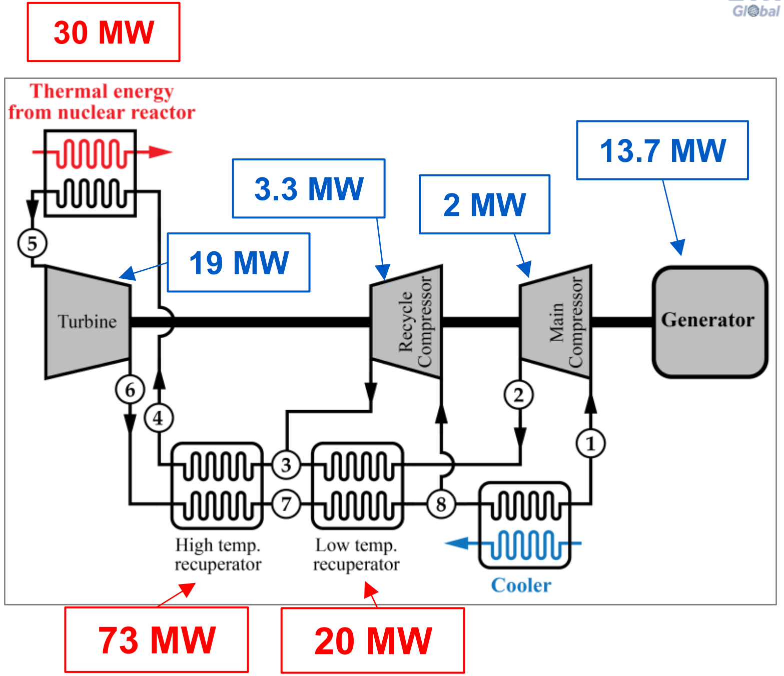
T-s diagram of power cycle



Exemplary power cycle layout for SMRs

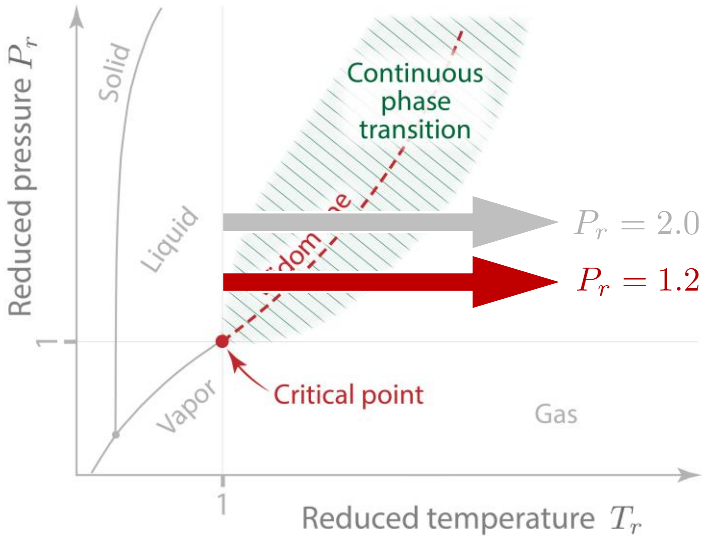
Motivation – Heat Transfer

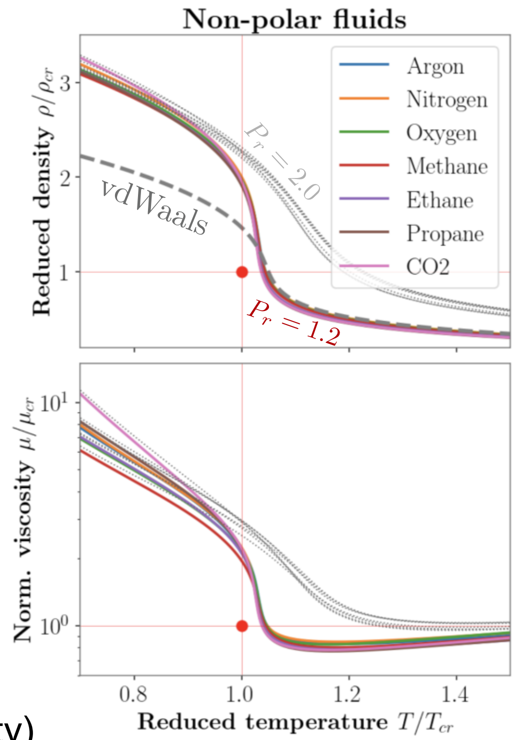
- Heat transfer dominates overall energy balance
- HTC and skin friction set heat transfer capacity and pressure loss
- **Overall pressure loss of 15 bar in all HEX and piping → 4% thermal efficiency drop**
- Small gains → large impact
- Accurate models needed



Exemplary power cycle layout for SMRs

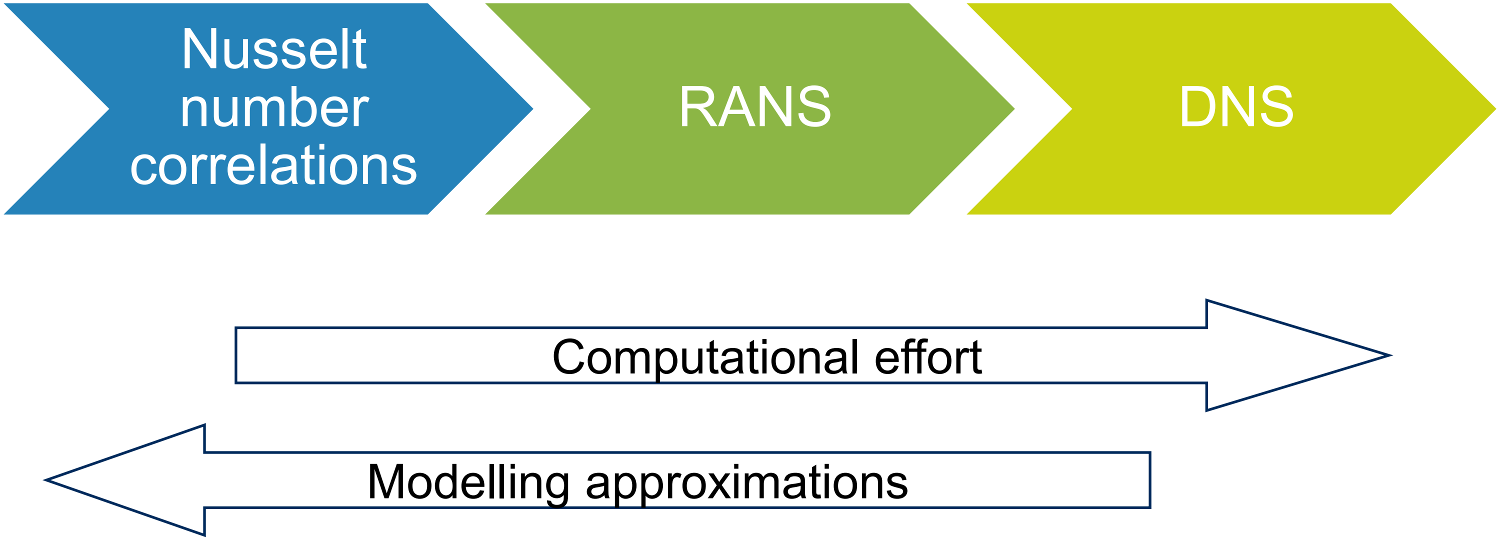
Thermophysical Properties





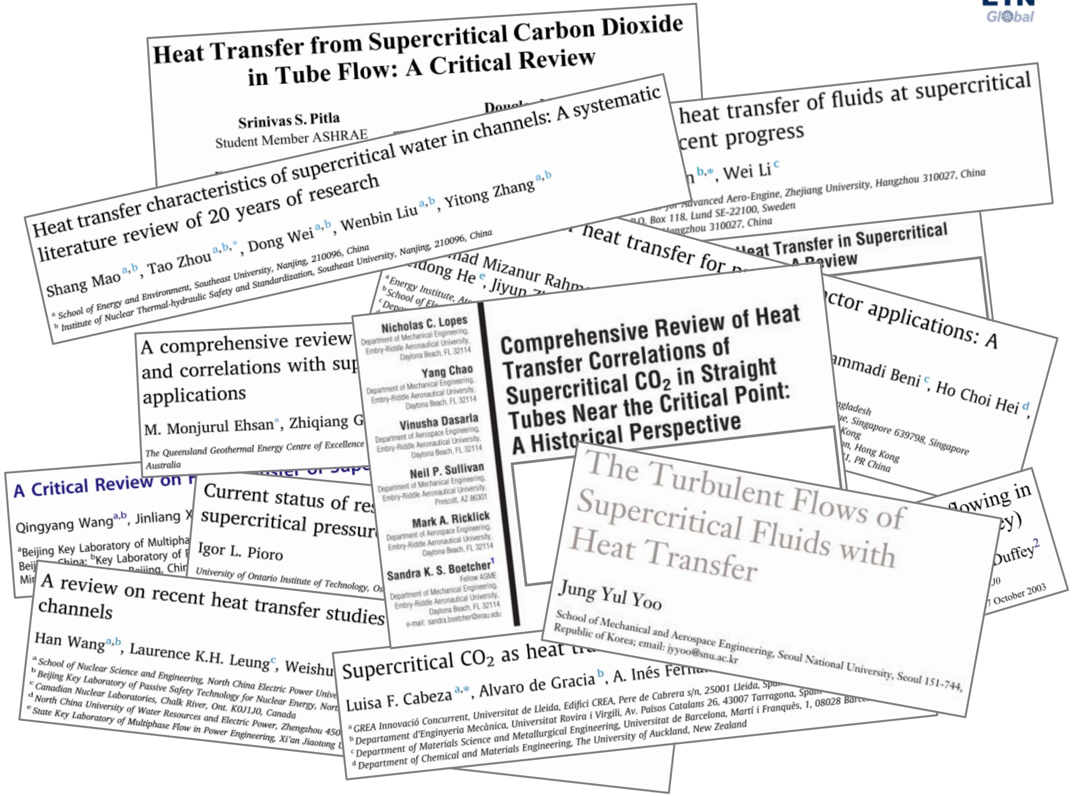
- Strong property variations across Widom line (pseudo-boiling)
- Nonpolar fluids show similar reduced-property trends (even viscosity) (VdW principle of corr. states)

Modelling Heat Transfer



Nusselt Number Correlations

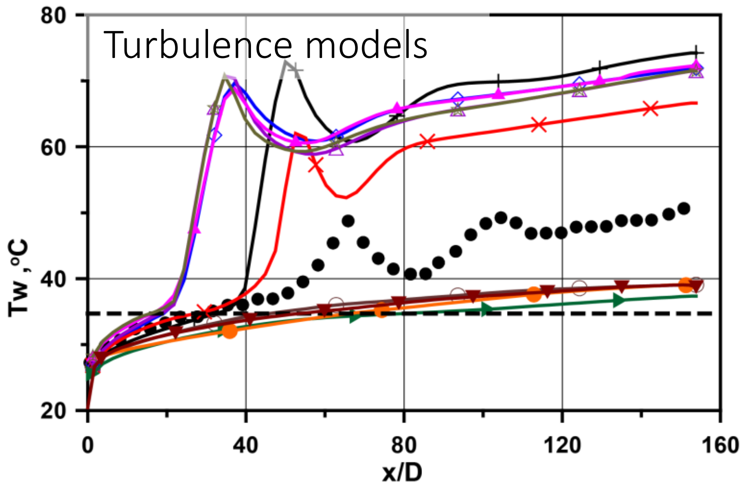
- Many different correlations (differing approaches, scaling laws, AI, proprietary/in-house, etc.)
- Orientation-specific buoyancy effects (vertical vs. horizontal arrangement)
- Built from narrow datasets (often nuclear thermal-hydraulics)
- Mostly steady-state
- High uncertainty outside design range (near - pseudocritical conditions need special care)



RANS (Reynolds Averaged Navier-St.)

- Turbulence model specific results (not predictive)
- Turbulence models are built on the **constant-property/incompressible law-of-the-wall**
- Models fail when property variations are present (even with ideal gases)

Heat transfer to sCO_2
Re = 3000 – 14000
Heat flux = 15-180 kW/m^2

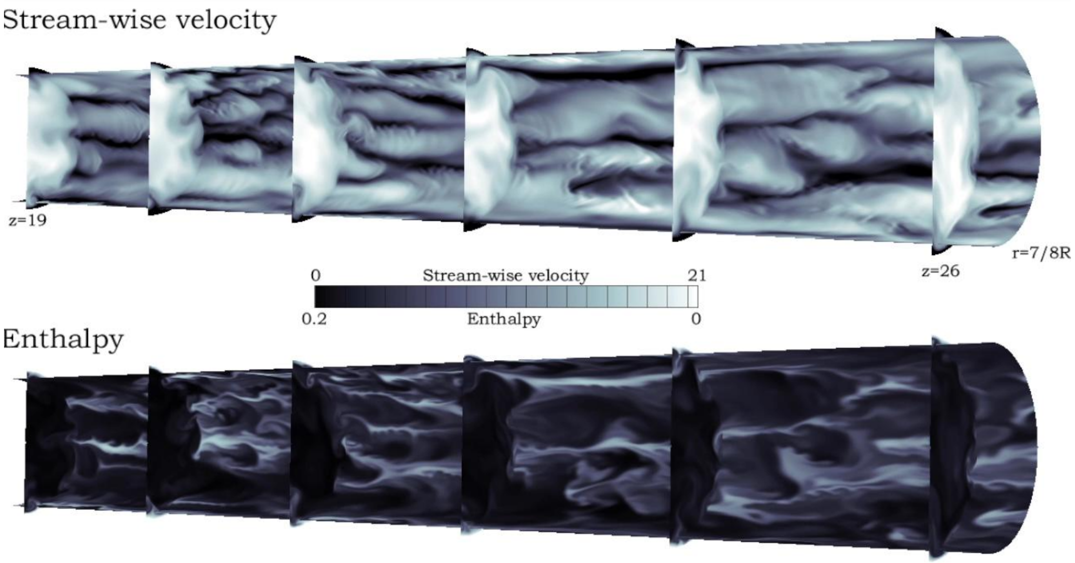


Sharabi, Ambrosini, Ann. Nuclear Energy

DNS (Direct Numerical Simulations)

- First-principles: resolves all time & length scales (no turbulence model)
- Computationally expensive: research only - not for day-to-day design
- Simple cases: channel/pipe/flat plate; smooth walls;
- Highest information content: “ground truth” → improve models

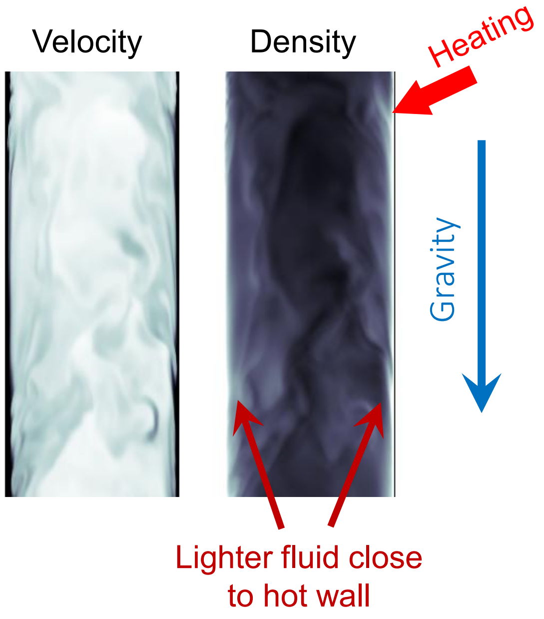
Pipe flow simulation with heated sCO_2



Nemati, Pecnik et al., JFM 2016
Peeters, Pecnik et al. JFM 2016

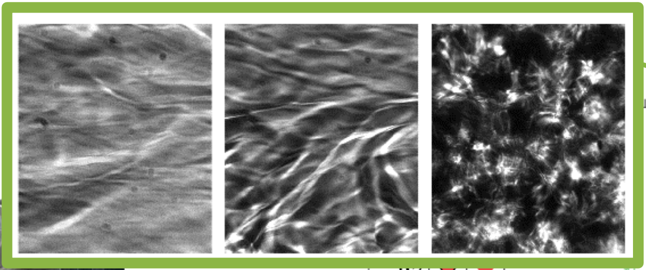
Key mechanisms to account for

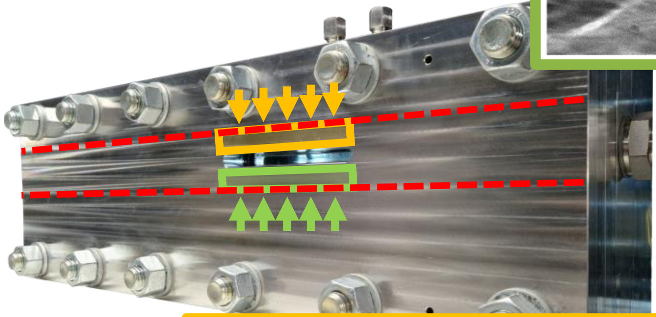
- **Thermophysical property variations**
  (viscosity, conductivity, isobaric heat capacity, density)
  - Apparent changes in heat transfer characteristics
- **Turbulence modulation by property variations**
  - Turbulence models must account for it
- **Buoyancy (vertical / horizontal flows)**
  - Direct effects: mean momentum affected by buoyancy
  - Indirect effects: turbulence affected by buoyancy
- **Flow acceleration due to thermal expansion**

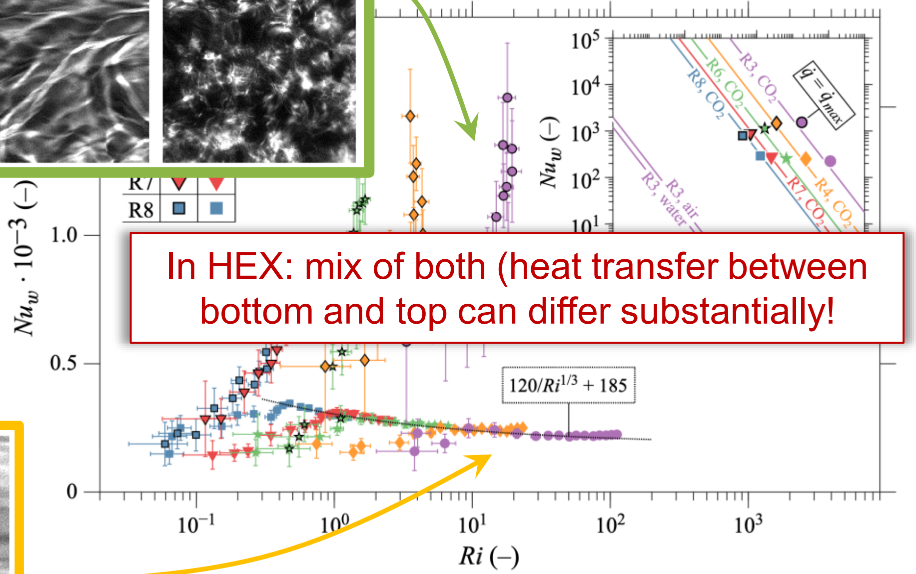


Buoyancy (horizontal flow)

Unstably stratified
(bottom heated)

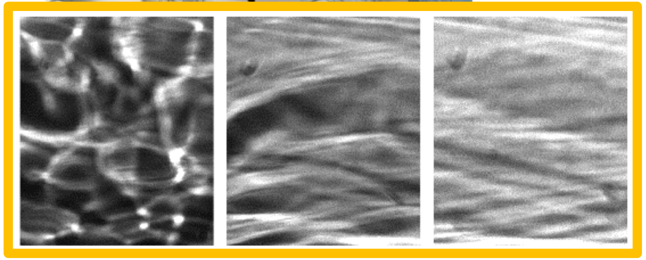






In HEX: mix of both (heat transfer between bottom and top can differ substantially!

Stably stratified
(top heated)



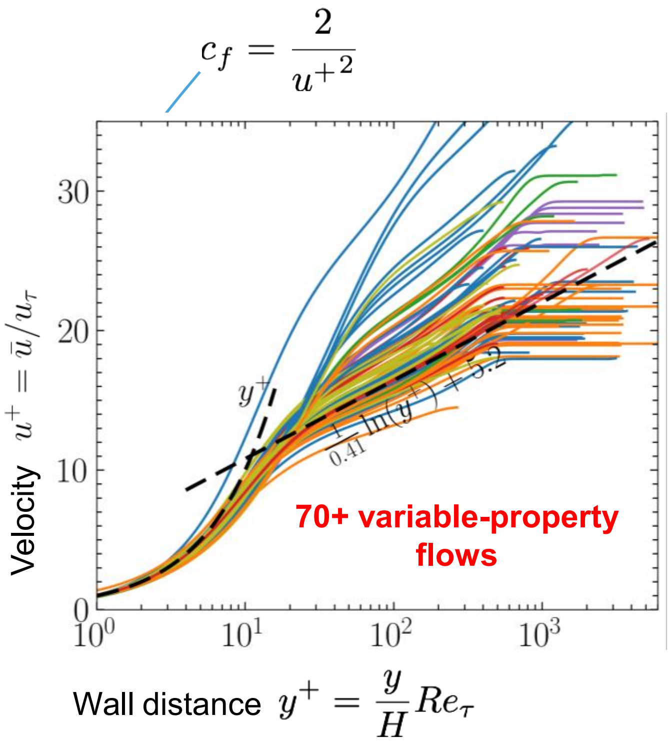
Buoyancy / Flow Shear

Draskic, Westerweel, Pecnik, JFM 2025

Turbulence modulation by property variations

- **Law-of-the-wall == cornerstone in fluid mechanics**
  - Used in correlations and turbulence models for CFD
  - Based on constant-properties / incompressible flows
  - **Variable property flows do not follow this law**

- **<u>Universal law-of-the-wall</u> to account for property variations!**
  - Allows to correct turbulence models for CFD
    (Patel, Pecnik et al. JFM 2016;
    Hasan, Elias, Menter, Pecnik, JFM 2025)



Example result with CFD

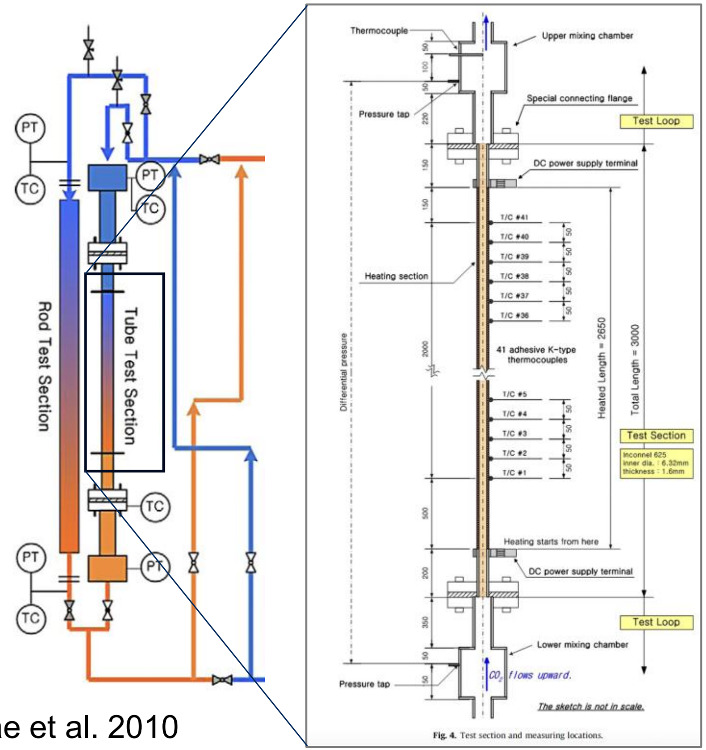
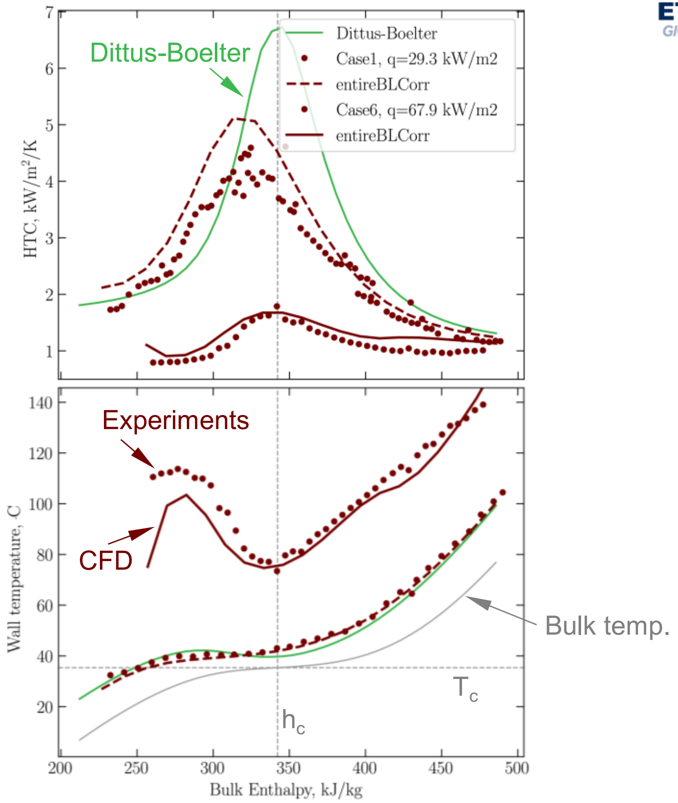


Fig. 4. Test section and measuring locations.

Bae et al. 2010



Conclusion and Future Research

- **Physics that matter**:
  - variable properties, buoyancy (orientation), and thermal acceleration
- **Correlations**:
  - useful within trained ranges; weak in transients, and for complex geometries
- **CFD (RANS)**:
  - can be predictive with property-aware corrections
- **Data gaps for validation**:
  - horizontal flows at high Ri (stable & unstable stratification), non-circular/compact channels, roughness, and transients
- **Next steps:**
  - open benchmarks, high-quality datasets

Back to Basics: Status of sCO_2 Fundamental Research

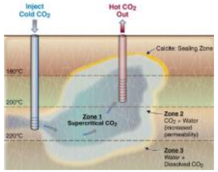
Material Compatibility

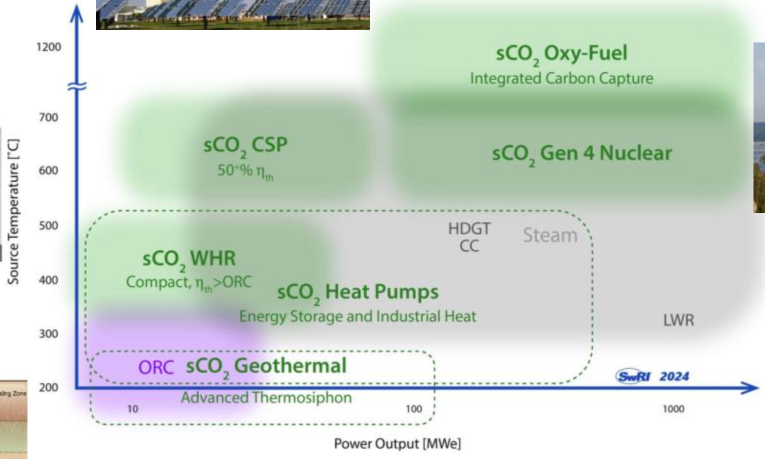
Henry Saari

sCO_2 Power Cycles

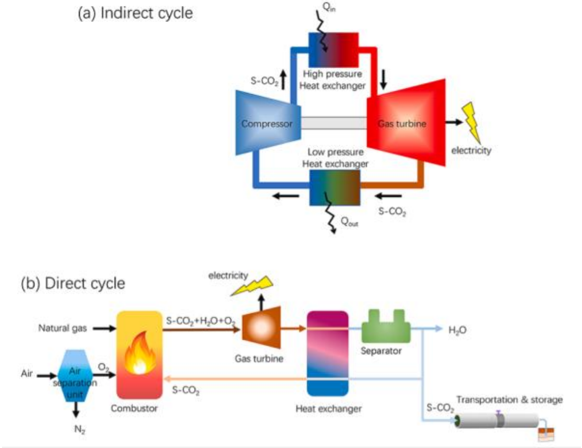
Heat Sources and Configurations

Many possible heat sources with various temperatures…indirect and direct cycle configurations with many different arrangements





sCO_2 power cycle heat sources [Hofer, 2024; Wilkes, 2024]



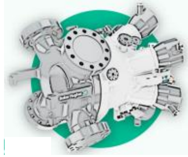
Schematics of (a) indirect and (b) direct cycles [Li, 2023]

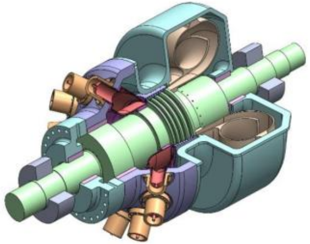
sCO_2 Power Cycles

Power Plants and Equipment

sCO_2 Brayton cycle technology overlaps that of steam and gas turbines, but they are unique systems for which material selection is especially critical

50 MW_{th} Demonstration Facility and turboexpander [NET Power, 2024]

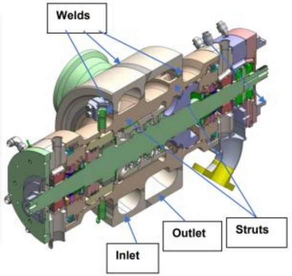




300 MW_e Oxy-fuel turbine concept [Moore, 2023]

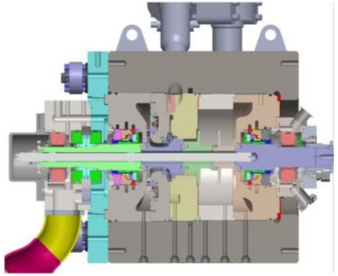
Turbine stop valve [Stevenson, 2024]

10 MW_e STEP Demo [Stevenson, 2024]



sCO_2 turbine [Stevenson, 2024]

PCHE high temperature recuperator [Stevenson, 2024]

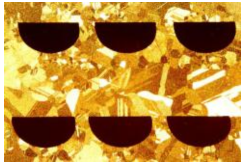


sCO_2 compressor [Cich, 2020]

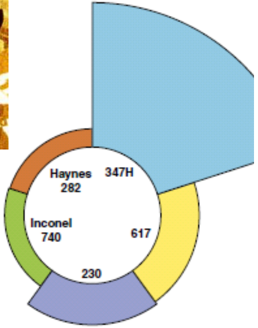
sCO_2 Power Cycles

Materials and Selection

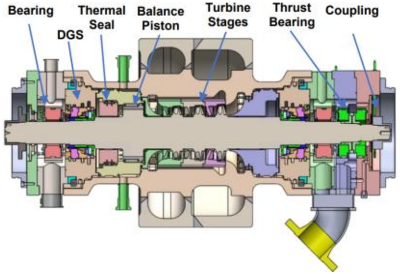
PCHE high temperature recuperator [Stevenson, 2024]



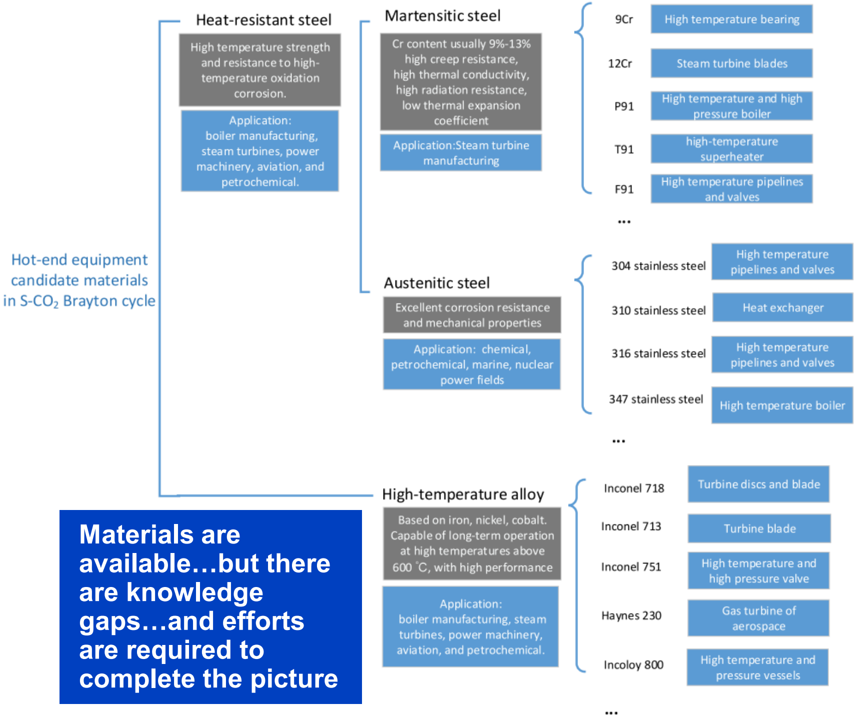
Micrograph of PCHE section [Southall, 2008]



Turbine stop valve [Stevenson, 2024]



STEP Turbine [Moore, 2024]



Materials are available…but there are knowledge gaps…and efforts are required to complete the picture

Materials options [Xu, 2023]

sCO_2 Corrosion

Fundamentals

CO_2 Corrosion at Elevated Temperatures

- Oxidation

$$xM + yCO_2 = M_xO_y + yCO$$

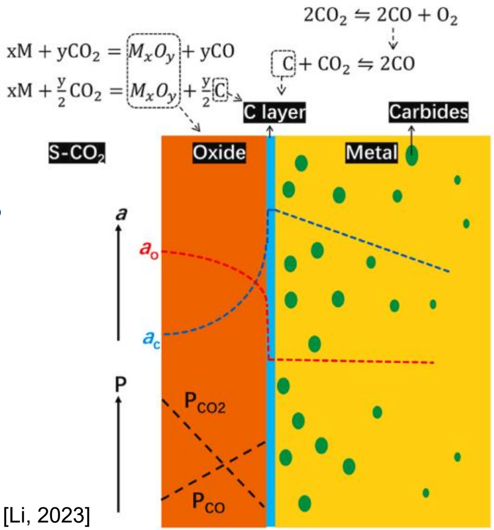
$$xM + (y/2)CO_2 = M_xO_y + (y/2)C$$

  - Oxygen partial pressure high enough to induce oxidation
  - Formation of oxide layer
- Carburization

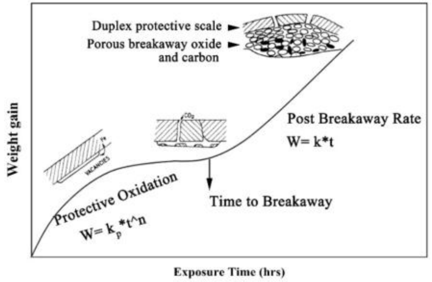
$$2CO_2 \leftrightarrow 2CO + O_2$$

$$2CO \leftrightarrow CO_2 + C$$

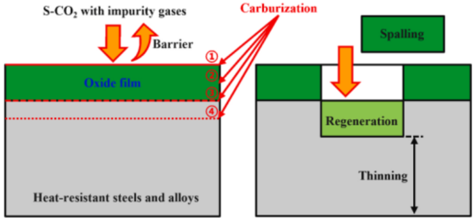
  - Penetration of C through the oxide layer
  - Reaction with metallic elements



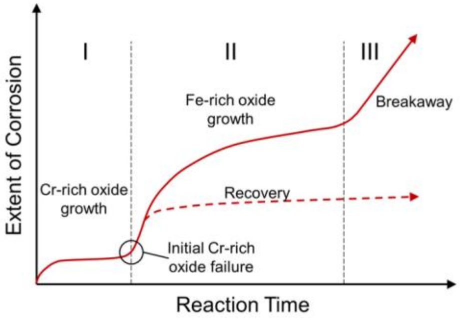
[Li, 2023]



[Zhang, 2025]



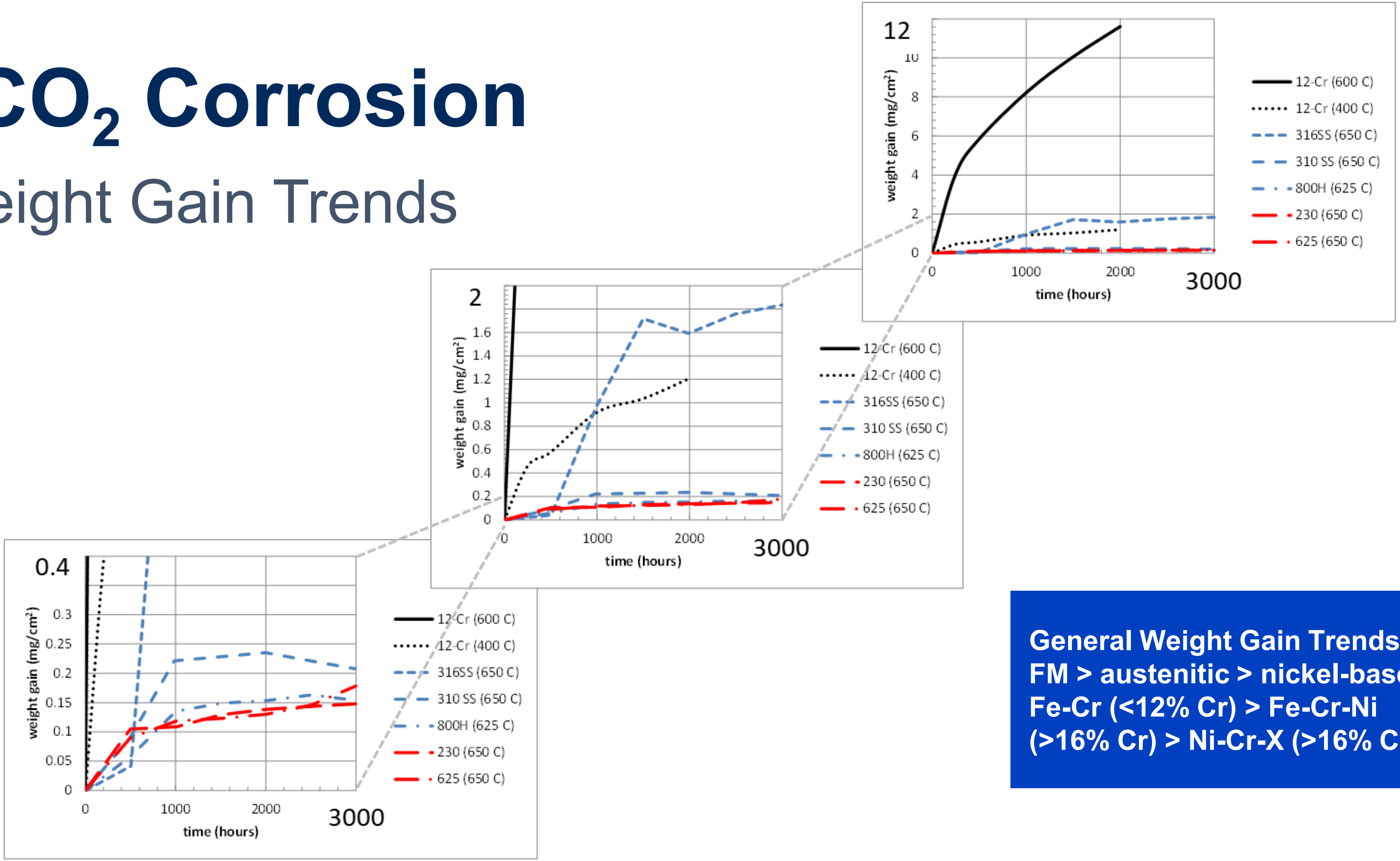
[Liang, 2025]



[Oleksak, 2020]

sCO_2 Corrosion

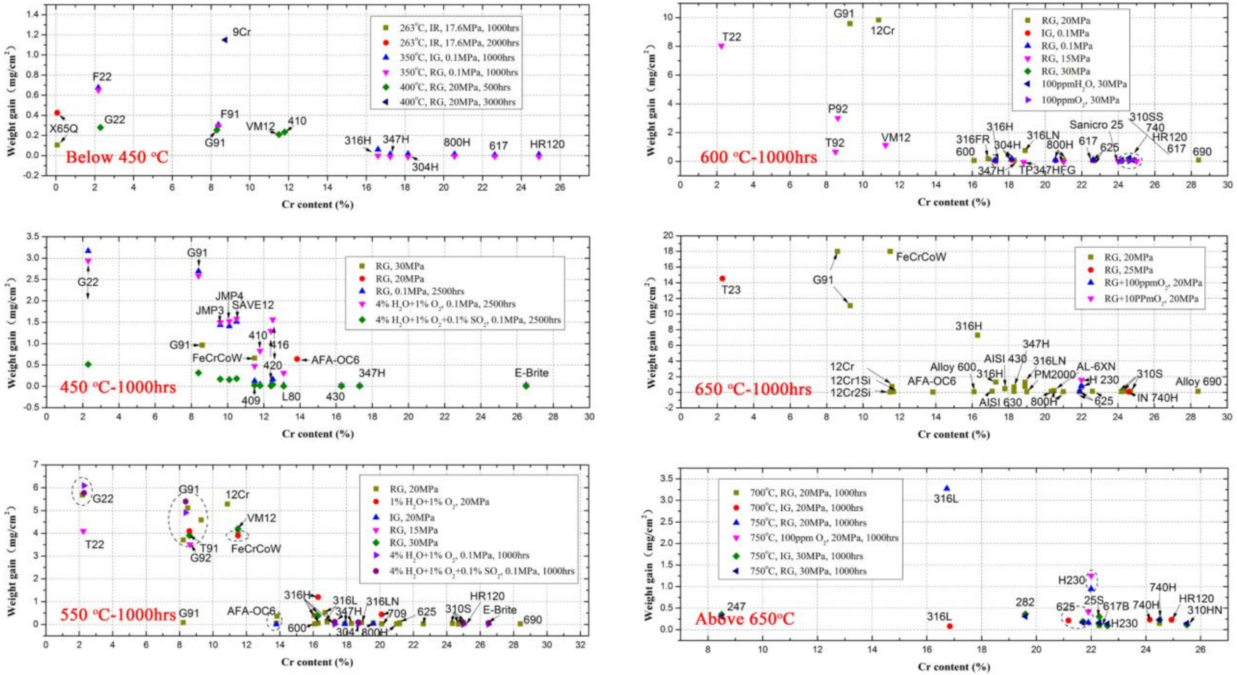
Weight Gain Trends



General Weight Gain Trends
FM > austenitic > nickel-base
Fe-Cr (<12% Cr) > Fe-Cr-Ni (>16% Cr) > Ni-Cr-X (>16% Cr)

sCO_2 Corrosion

Weight Gain Trends



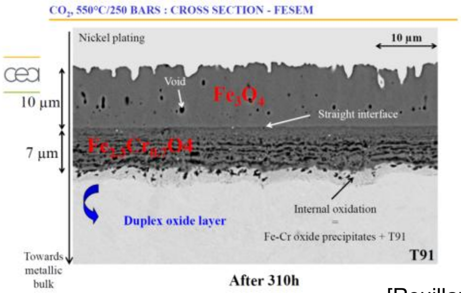
General Weight Gain Trends
FM > austenitic > nickel-base
Fe-Cr (<12% Cr) > Fe-Cr-Ni (>16% Cr) > Ni-Cr-X (>16% Cr)

Results depend on temperature, pressure, presence of impurities, alloying

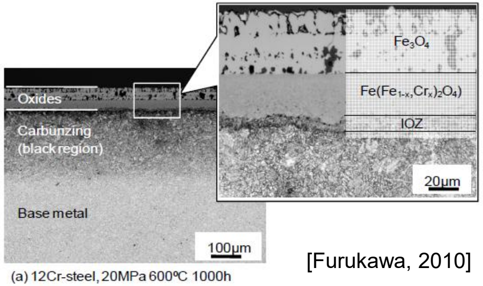
Weight gain data versus Cr content of various alloys under various testing conditions [Zhang, 2025]

sCO_2 Corrosion

Scales – Ferritic-Martensitic Steels



[Rouillard, 2011]



[Furukawa, 2010]

T91 9Cr F-M steel

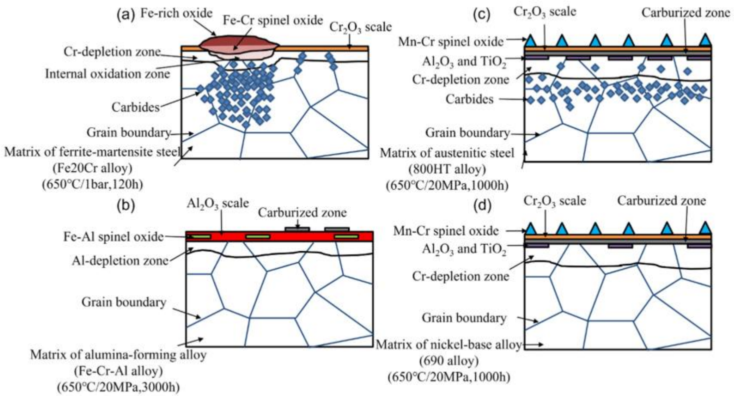
- Duplex oxide layer
  - Outer: magnetite, Fe_3O_4
  - Inner: spinel, $Fe_{3-x}Cr_xO_4$
- Internal oxidation also
- Extrapolation to 20 years
  - Corrosion layer thickness = 500 µm

12Cr Martensitic steel

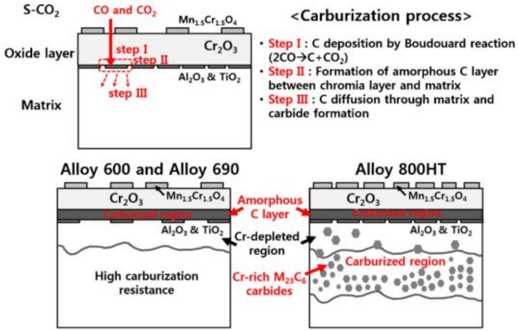
- Two successive layers, no breakaway corrosion
  - Outer: Fe oxide, Fe_3O_4
  - Inner: Fe+Cr oxide, $Fe(Fe_{1-x},Cr_x)_2O_4$
- Thin internal oxide zone (IOZ) between base metal and inner layer
- Carburizing observed near surface in base metal
  - Factor in breakaway corrosion, degradation of ductility

sCO_2 Corrosion

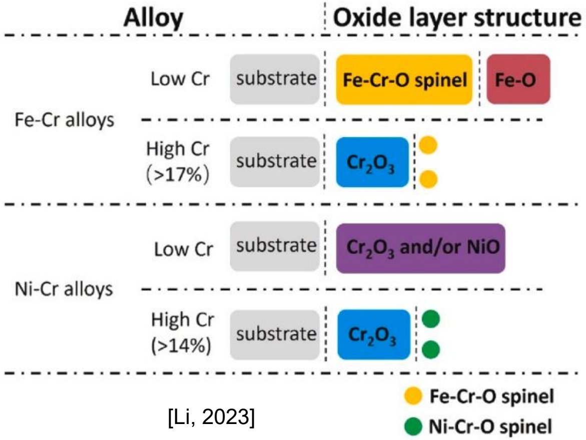
Scales – Various Alloy Systems



(a) FM steel (b) AFA (c) austenitic steel (d) nickel-base alloy [Yang, 2022]

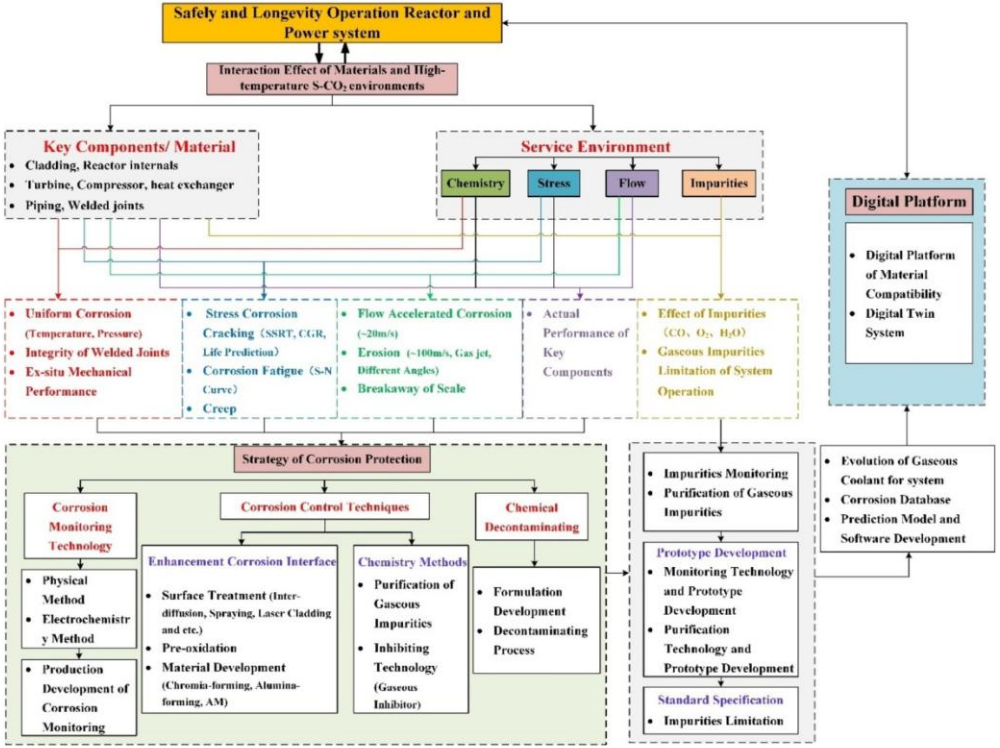


Oxide formation and carburization process for nickel-base alloys and 800 HT [Lee, 2015]



[Li, 2023]

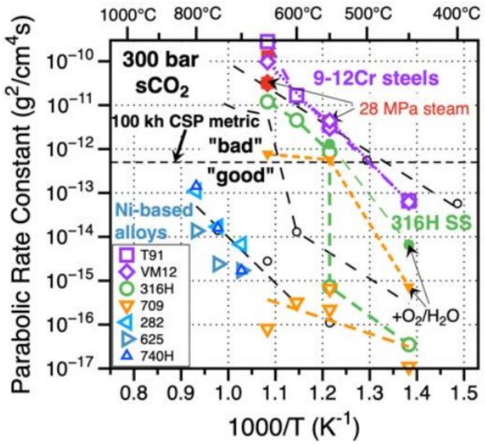
sCO_2 Corrosion – Current Research



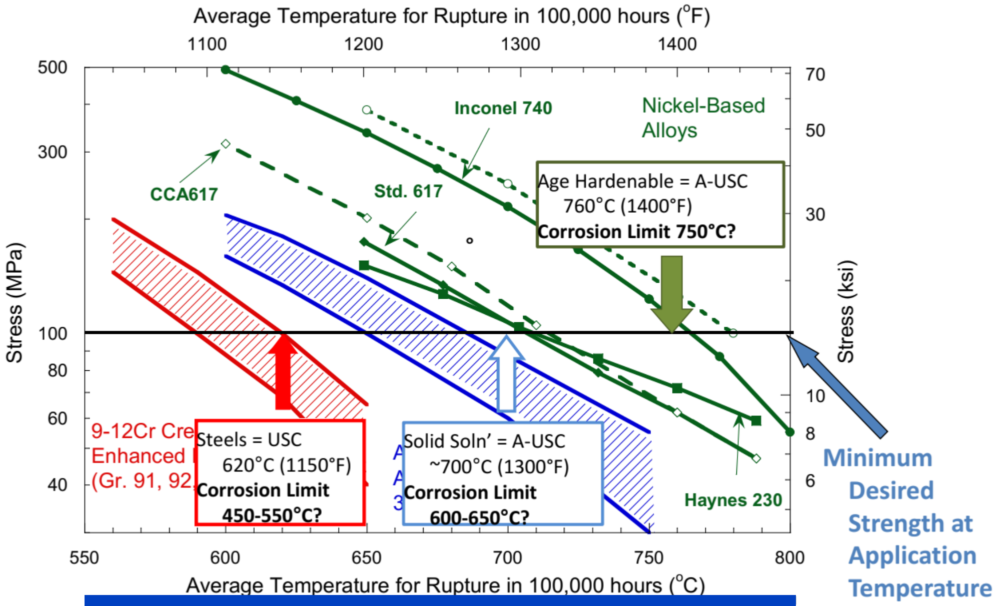
Overview of current research on sCO_2 materials corrosion [Zhang, 2025]

sCO_2 Materials Selection

Strength and Corrosion



Summary of corrosion rate constants for various alloys and conditions, compared to CSP-developed metric for 100 kh life [Pint, 2024]



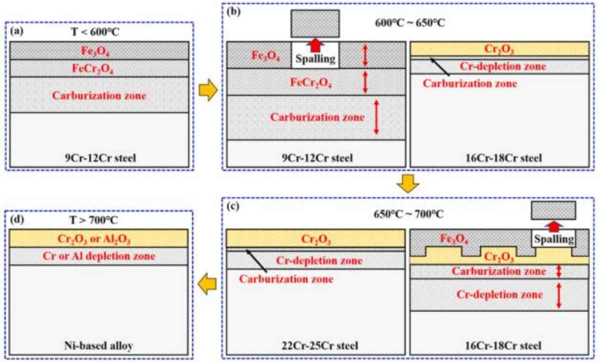
Where are the temperature cut-off for different materials when corrosion is considered?

sCO_2 Materials Selection

Strength and Corrosion

Recommended maximum working temperature of Fe- and Ni-based alloys as candidate materials for different components in $S\text{-}CO_2$ environments.

Alloy type		Typical alloys	Recommended temp. (°C)	Notes
Fe-based	Low Cr ferritic steels	T22	<450	
	High Cr ferritic steels	T/P91, T/P92, T/P122, HCM12A	<550	
	AFA	OC6, OC7, OC10, MA957	<550	Up to 650 °C for some AFAs with Cr > 20%.
	Austenitic stainless steels (Cr < 20%)	TP347HFG, Super SS304H, SS316,	<620	
	Austenitic stainless steels (Cr > 20%)	Alloy 800, SS310	<650	
Ni-based	Cr > 14%	Alloys 230, C-276, 282, 740, 617, 600, 690, 625	<750 °C or other severe environments (high contents of impurities)	For crucial parts like turbine, recommending Cr > 22%;Alloy 625 could be welding fillers.



[Liang, 2025]

Recommended temperature ranges	Alloy type	Typical alloys	Max Temperature Limit (°C)	Allowable Stress (MPa)
<350 °C	Low Cr Ferritic steels	T22	580	/
<450 °C	Martensitic Steels (9Cr)	T/P/F91	649	482 °C: 131.7 510 °C: 122.7
		T/P92	649	482 °C: 138.6 510 °C: 132.4
		T/P911	621	482 °C: 138.6 510 °C: 131.0
<500 °C	Martensitic Steels (12Cr)	T/P122	649	482 °C: 140.0 510 °C: 134.4
<600 °C	Austenitic steels (low Cr)	316	700	600 °C: 65 650 °C: 50
		347H	816	500 °C: 125
<650 °C	Austenitic steels (high Cr)	800H	816	500 °C: 138
		310	816	500 °C: 116
		HR120	899	500 °C: 113
		NF709	/	/
<700 °C	Solid solution strengthened nickel-based alloys	625	649	500 °C: 192
		617	982	750 °C: 50.4
		230	982	750 °C: 50.8
<750 °C	Precipitation strengthened nickel-based alloy	282	800	750 °C: 105
		740H	800	750 °C: 84.1

Recommended maximum use temperatures of different alloys for sCO_2 power cycles [Zhang, 2025]

sCO_2 Materials

Summary of Recent Results

<u>Mechanical Properties</u>

- Existing ASME code (and other) alloys OK
- Strength increases:
  - Ferritic –Austenitic – Ni-base
- Temperature capability may be limited/reduced by compatibility (corrosion/carburization)

<u>Compatibility</u>

- Extensive data are useful (more required?)
- Materials for AUSC, gas turbines +/- OK for sCO_2 applications
- Corrosion resistance increases:
  - Ferritic – Austenitic – Ni-base

<u>Long-term Behaviour</u>

- Many factors affect materials degradation and mechanical property changes
- Longer-term testing, results, and experience required under
  - Real operating conditions
  - Actual component shapes and forms

<u>Lessons Learned/to be Learned</u>

- Previous loops
  - Sandia National Laboratories
    - Piping, erosion
  - Naval Nuclear Laboratory
    - Erosion
  - Others?
- NET Power La Porte Test Facility
  - Open-cycle process demonstrator
- STEP
  - Materials availability, processing, fabrication
  - Compatibility with service environment
  - Operation under “real” conditions – flow, stress, etc.
  - Failures – failures modes, analysis

Overall Summary

Component	Component	Conditions (Indirect)		Codes/Tech Base	Materials	Temperature Limits	Tech Level
		T (°C)	P (bar)				
Low temperature	Piping Valves Heat exchangers	40-200	80-275	ASME B31.1 Power Piping, ASME B16.34 Valves, ASME BPVC Various supporting, USC	Low Cr ferritic (T22) Higher Cr ferritic (T/P91, T/P92) High Cr ferritic (T/P122)	<350-400 °C <400-500 °C <500-550 °C	High TRL Long-term compatibility under operating conditions?
High temperature	Piping Valves Heat exchangers	200-750	80-275	ASME B31.1 Power Piping, ASME B16.34 Valves, ASME BPVC Various supporting, A-USC	Austenitic SS (<20% Cr) Austenitic SS (>20% Cr) Ni-base	<600 °C <650 °C <750 °C	High TRL for SS Long-term compatibility under operating conditions? Low-medium TRL for Ni-base Long-term compatibility under operating conditions?
Compressor	Casing Impeller + shaft	40-200	80-275	OEMs Industrial Process Compressors	Steel casting Alloy steel forgings	Low Low	High TRL Degradation of soft seal materials?
Turbine	Casing Disks Blades	600-750	80-275	OEMs Gas and Steam Turbines, A-USC	Ni-base casting Ni-base forging Ni-base casting, integral forge + machine	<750 °C	Low-medium TRL Long-term compatibility? High TRL Long-term compatibility? High TRL Long-term compatibility?

sCO_2 Materials Review Papers

R. P. Oleksak and F. Rouillard, 4.14 – Materials Performance in CO_2 and Supercritical CO_2, in Comprehensive Nuclear Materials 2nd edition, Volume 4, pp. 422-451, 2020. (https://doi.org/10.1016/B978-0-12-803581-8.11622-4)

M. T. White, G. Bianchi, L. Chai, S. A. Tassou, A. I. Sayma, Review of supercritical CO_2 technologies and systems for power generation, Applied Thermal Engineering, Volume 185, 2021, 116447. (https://doi.org/10.1016/j.applthermaleng.2020.116447)

Kaiyang Li, Zhongliang Zhu, Bo Xiao, Jing-Li Luo, Naiqiang Zhang, State of the art overview material degradation in high-temperature supercritical CO_2 environments, Progress in Materials Science, Volume 136, 2023, 101107. (https://doi.org/10.1016/j.pmatsci.2023.101107)

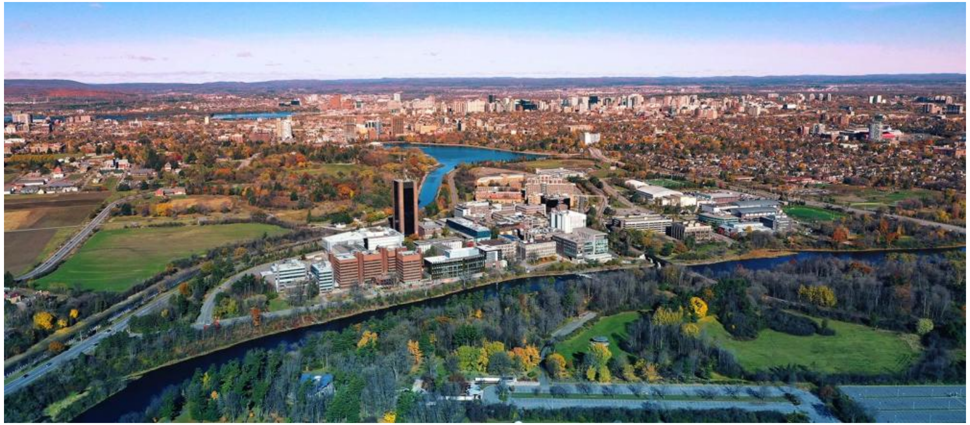
Z. Xu, Y. Yang, S. Mao, W. Wu, Q. Yang, Review on corrosion of alloys for application in supercritical carbon dioxide brayton cycle, Heliyon, Volume 9, Issue 11, 2023, e22169. (https://doi.org/10.1016/j.heliyon.2023.e22169)

B. A. Pint, R. Pillai, J. R. Keiser, Summary of structural alloy compatibility in supercritical CO_2 at 450°-800°C, Advances in Materials, Manufacturing, and Repair for Power Plants: Proceedings from the Tenth International Conference, October 15-18, 2024, Bonita Springs Florida, USA. (https://doi.org/10.31399/asm.cp.am-epri-2024p0885)

M. C. Galetz, E. M. H. White, M. Kerbstadt, C. Schlereth, X. Montero, D. Benitez, Material Challenges and Alloy Selection for Particle/s-CO_2 Heat Exchangers in Concentrated Solar Power Systems, Advanced Engineering Materials, Volume 27, Issue 10, 2025, 2402060. (https://doi.org/10.1002/adem.202402060)

Z. Liang, T. Guo, Q. Zhao, A review of corrosion and protection of alloys in supercritical carbon dioxide power cycles: From the perspectives of corrosion simulation, dynamic simulation to experimental research, The Journal of Supercritical Fluids, Volume 224, 2025, 106647 (https://doi.org/10.1016/j.supflu.2025.106647)

Zhang G, Huang Y-P, Zhao Y-F, et al. High-temperature oxidation and carburization, corrosion protection, materials selection and coolant chemistry for supercritical carbon dioxide power cycles: A review. International Materials Reviews. 2025;0(0). (https://doi.org/10.1177/09506608251369099)



Thank you for your attention

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Thank you and see you next time!

Question / comments?

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