

Mixing it up: the effect of dopants on the design of CO₂ cycle and turbine

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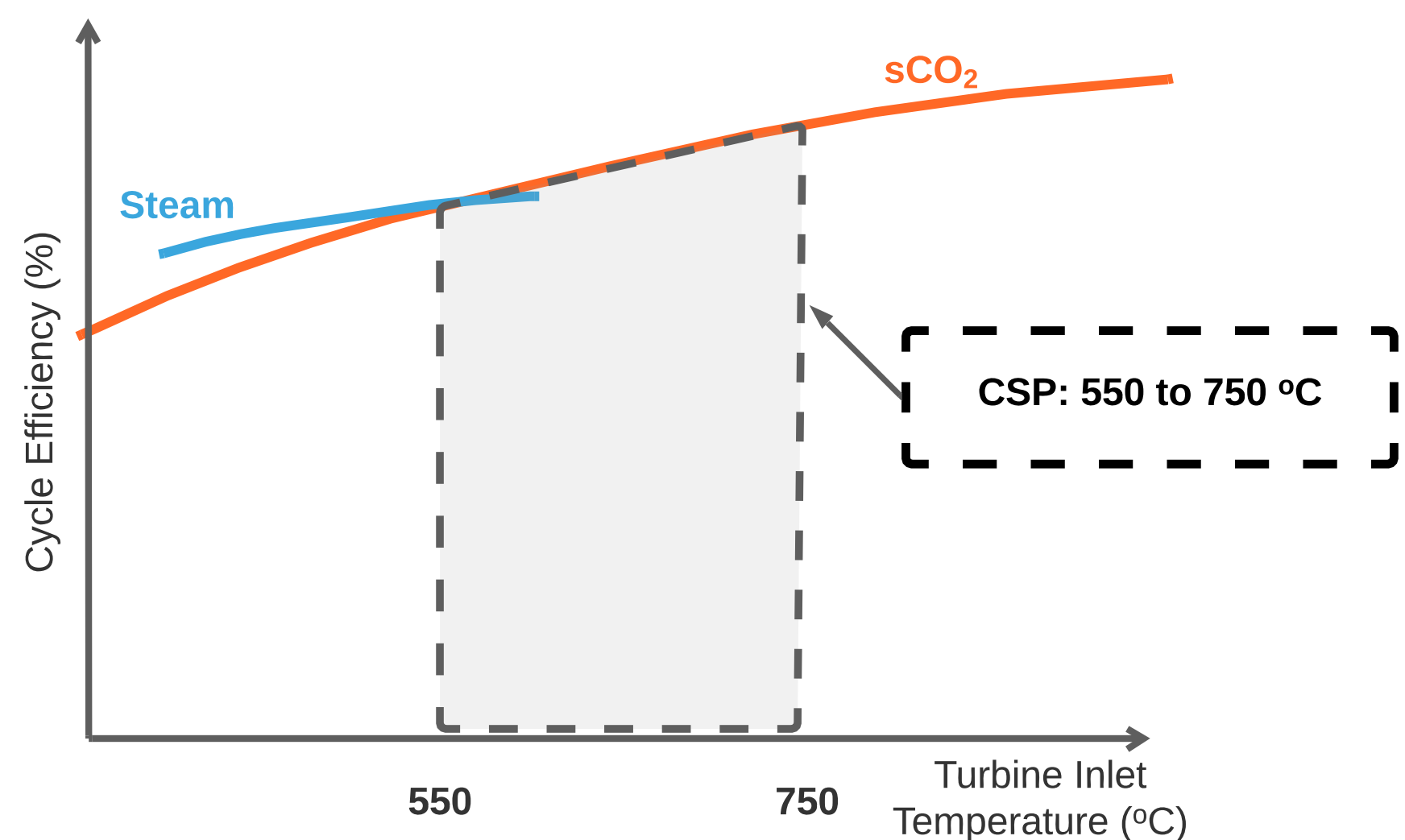
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Technological context

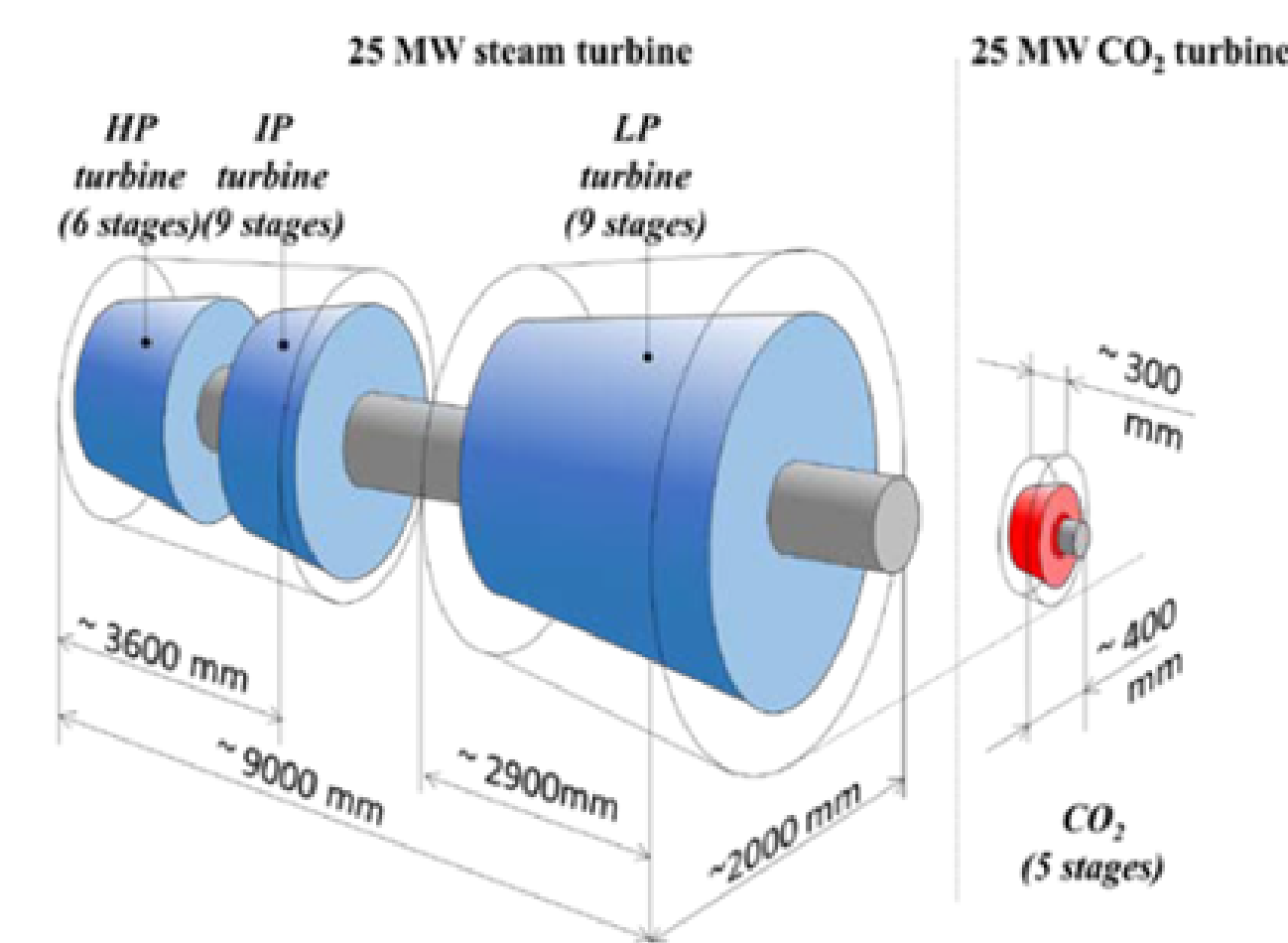
Supercritical CO₂ cycles

Supercritical carbon dioxide (sCO₂) was identified as a viable working fluid for power plants as early as the 1960's. Research has shown that it may outperform state-of-the-art steam cycle for turbine inlet temperatures >550 °C, which makes it a valuable asset for advanced concentrated solar power (CSP)



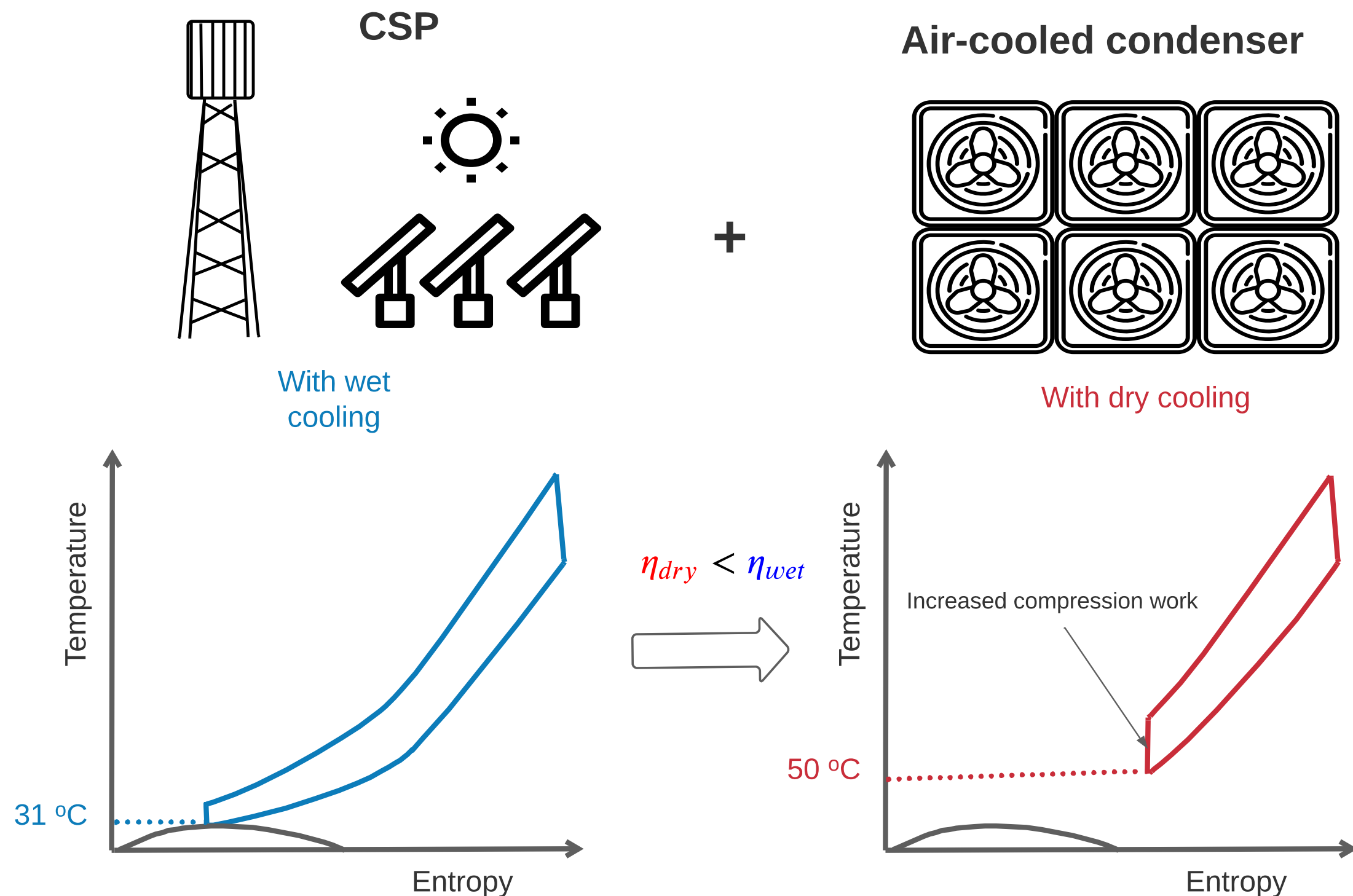
Why CO₂?

- Abundant
- Cheap
- Non-toxic
- Non-flammable
- Thermally stable at high temperatures
- Good cycle efficiency
- Compact turbomachinery



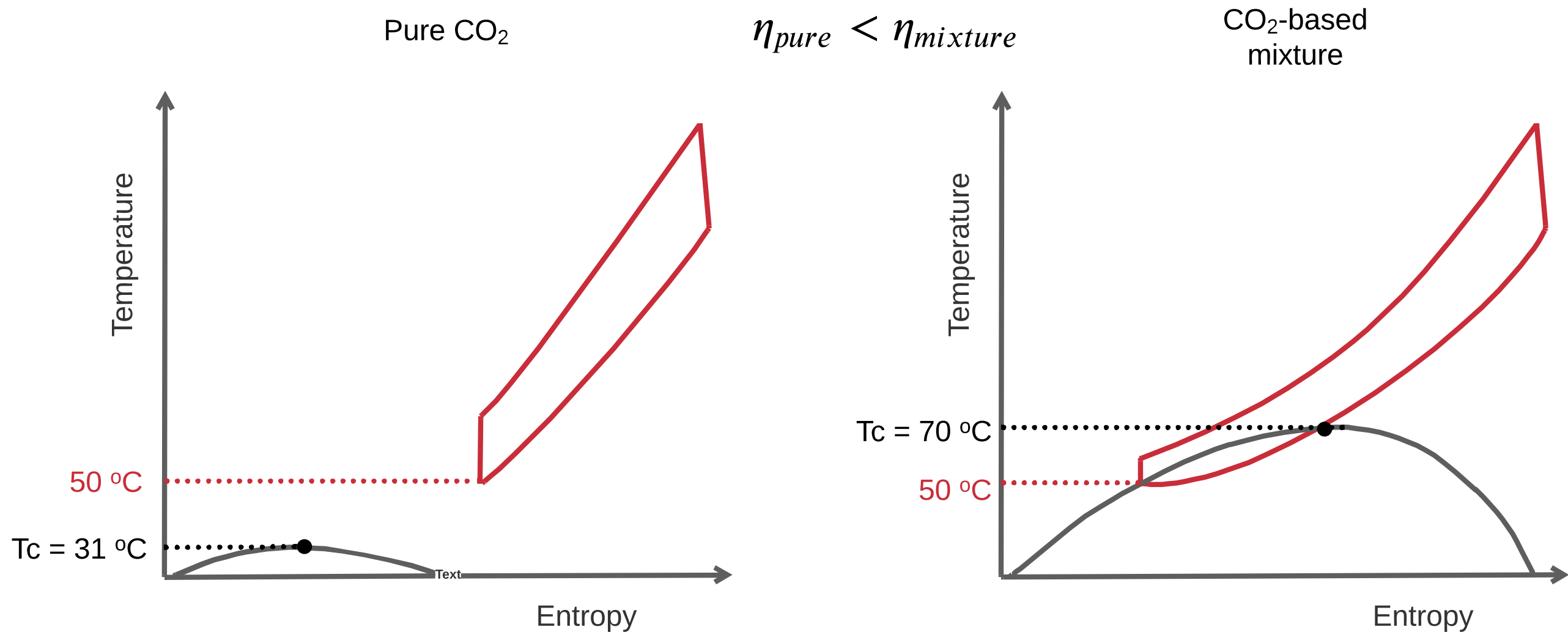
Challenges

CSP built in arid locations do not have access to cooling water, therefore need to depend of ambient air for cooling. This leads to higher compression work and reduced efficiency since the fluid will be compressed at higher temperatures (40 to 50 °C)

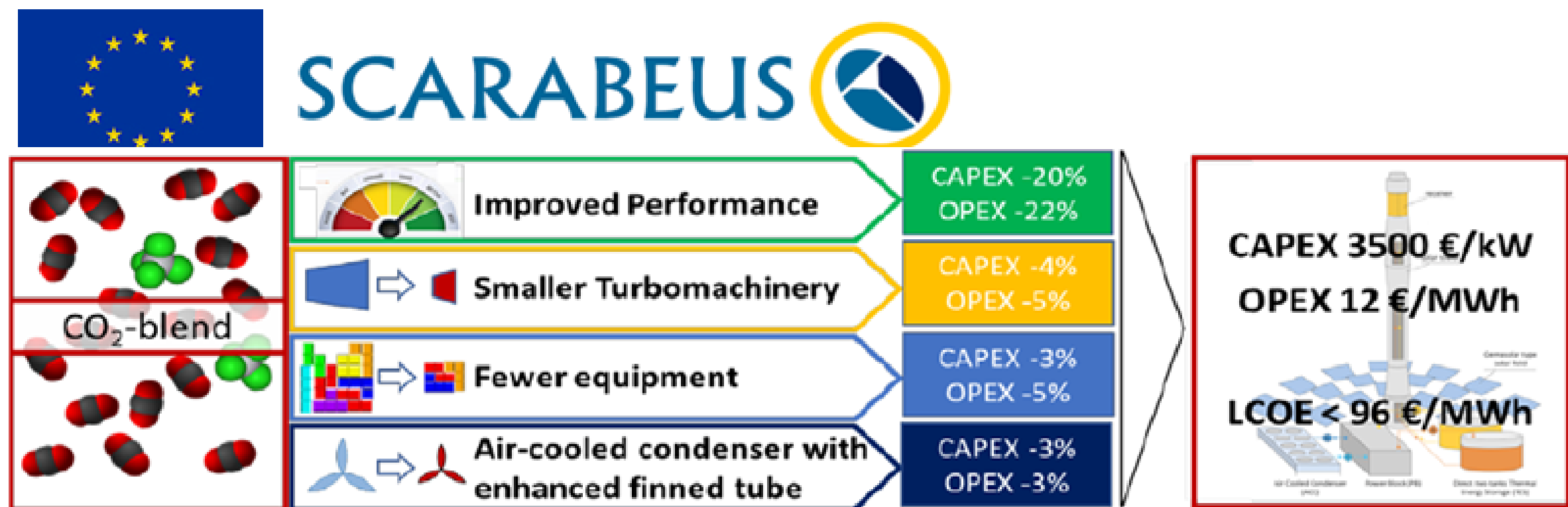


Solution

Increasing the critical temperature of CO₂ by adding impurities (dopants) makes the cycle more compatible with dry cooling temperatures and allows for working fluid condensation. This reduces compression work and increasing thermal efficiency.

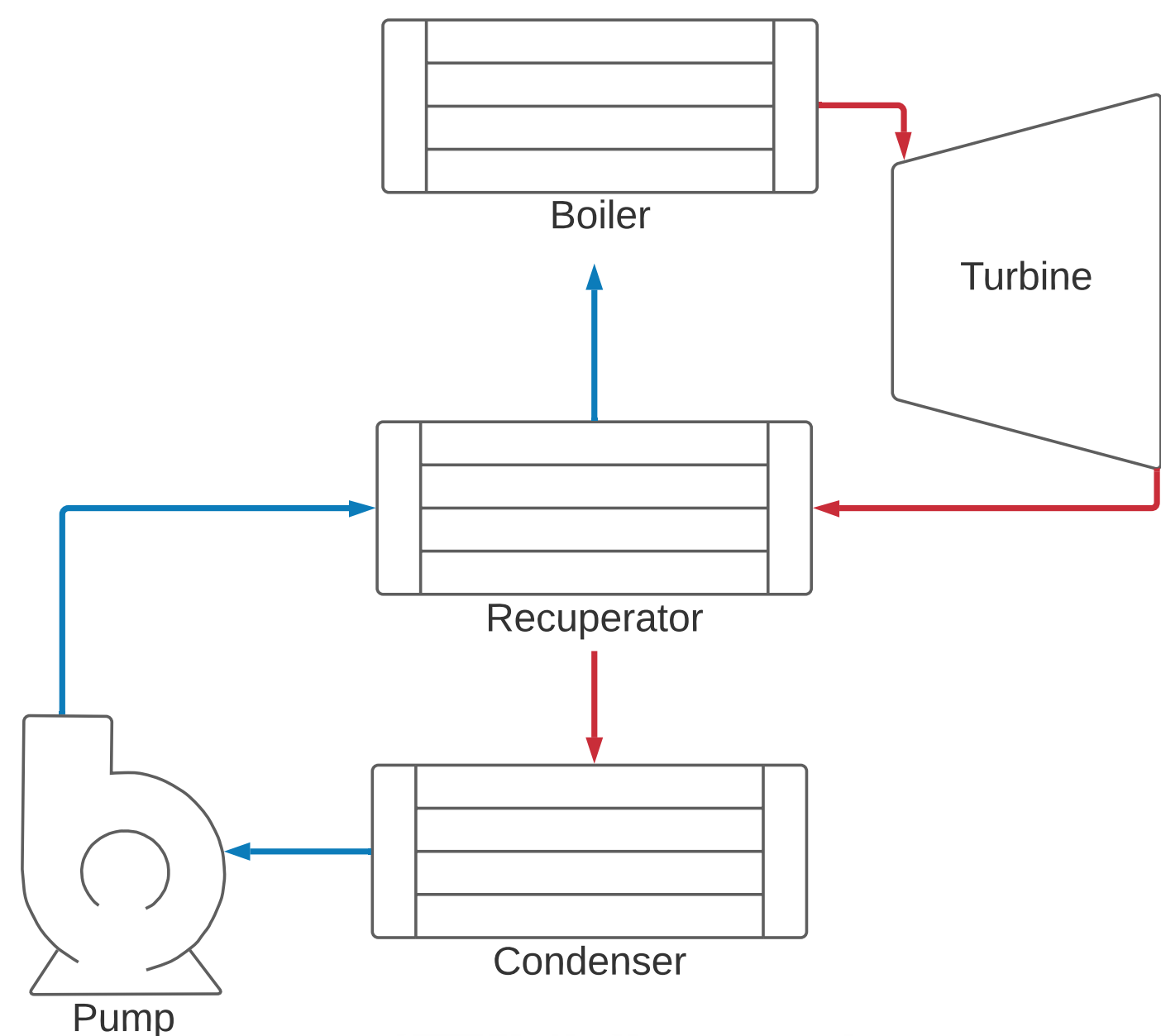


The SCARABEUS project aims to identify the best dopant type and amount that will result in the lowest levelised cost of electricity (LCOE) for CSP plants employing dry cooling.



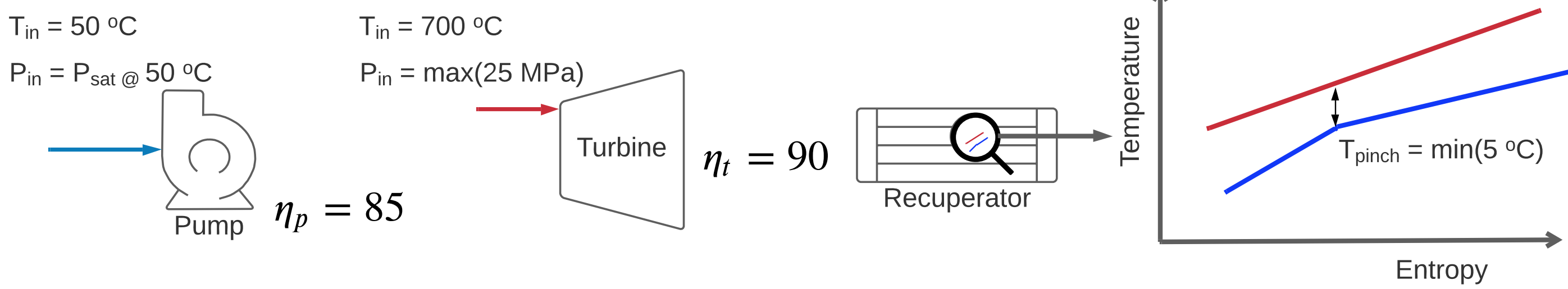
Methodology

A MATLAB code was developed to model a simple recuperated cycle.

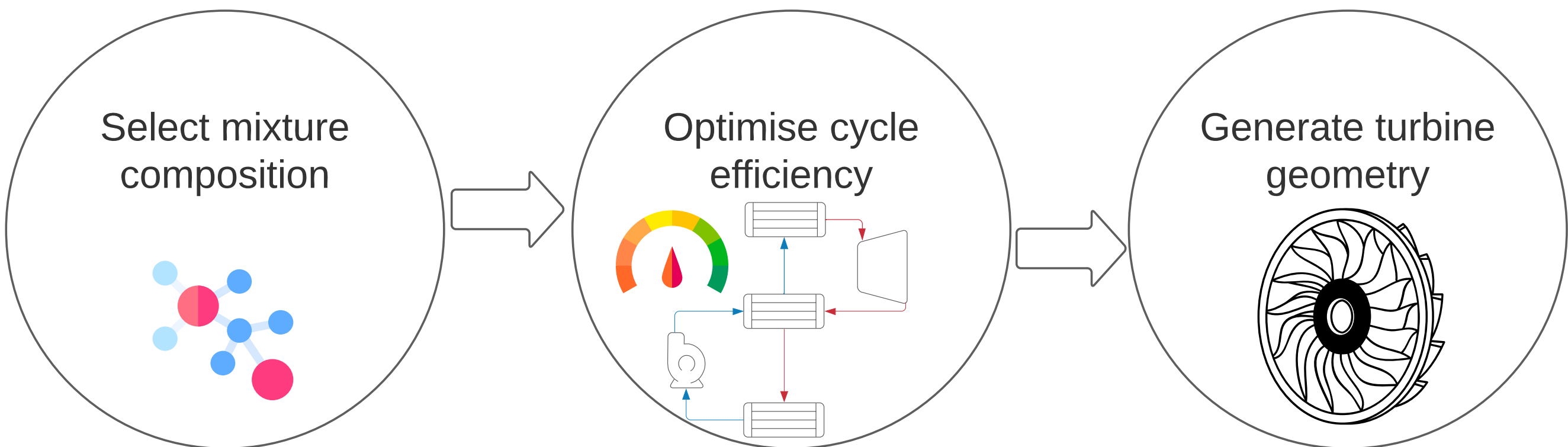


Matlab

Cycle optimisation parameters:



To test the effect of the dopant amount on the cycle and turbine design, the cycle optimisation study is repeated for each dopant molar fraction. A turbine geometry is then generated based on the boundary conditions imposed by the optimal cycle conditions.



A case of **100 MW** capacity power plant was modelled to demonstrate the effect of dopants on a four-stage axial turbine geometry.

Working Fluid modelling:

Three dopants were studied based on recommendations by the SCARABEUS project:

- Titanium tetrachloride (TiCl₄)
- Sulphur dioxide (SO₂)
- Hexafluorobenzene (C₆F₆)

A 3rd party software, Simulis Thermodynamics, was employed to model the working fluid and calculate its properties at each point in the cycle. Within Simulis, the Peng-Robinson (PR) equation of state was used in conjunction with the Van der Waals (VdW) mixing rules.



PR EoS:

$$P = \frac{RT}{v-b} - \frac{aa}{(v^2+2bv-b^2)}$$

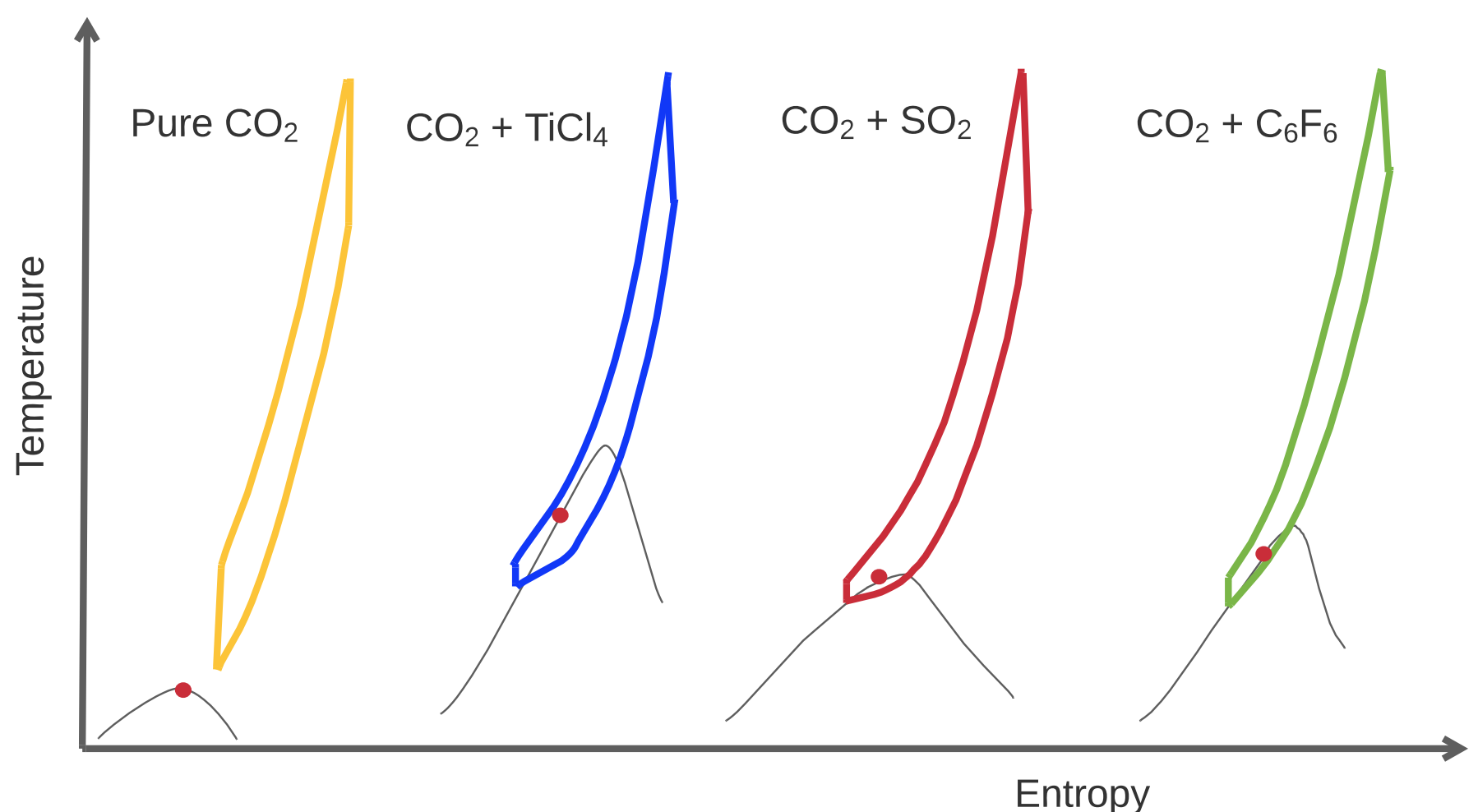
VdW mixing rules:

$$a = \sum_i^N \sum_j^N x_i x_j a_{ij}$$
$$b = \sum_i^N \sum_j^N x_i x_j b_{ij}$$

Results

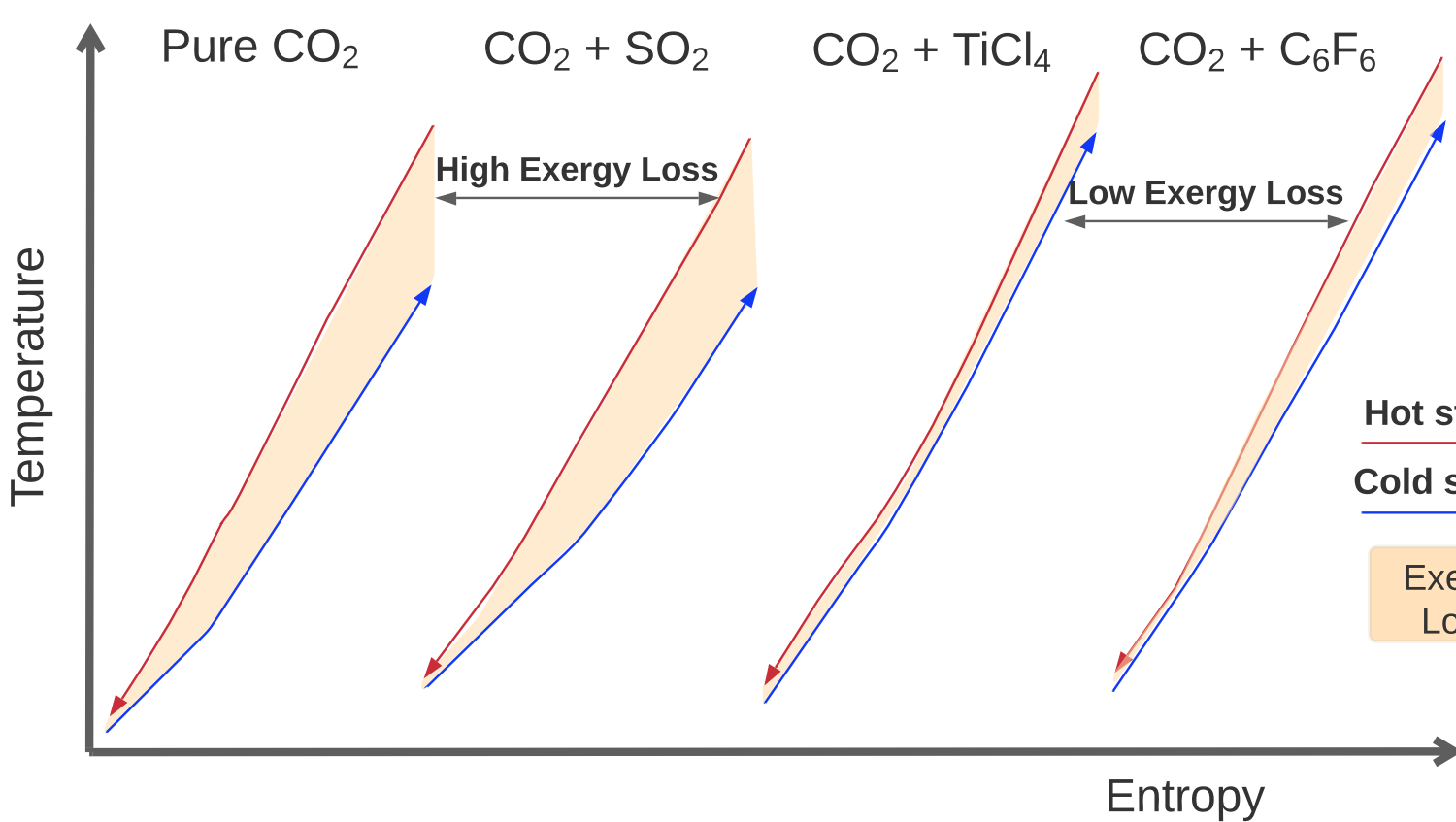
Cycle Analysis:

Working fluid	Dopant molar fraction	Critical temp. (°C)	Cycle efficiency (%)
Pure CO ₂	0	31	41.7
CO ₂ + TiCl ₄	0.174	104	49.5
CO ₂ + SO ₂	0.264	54	42.3
CO ₂ + C ₆ F ₆	0.167	87	46.5

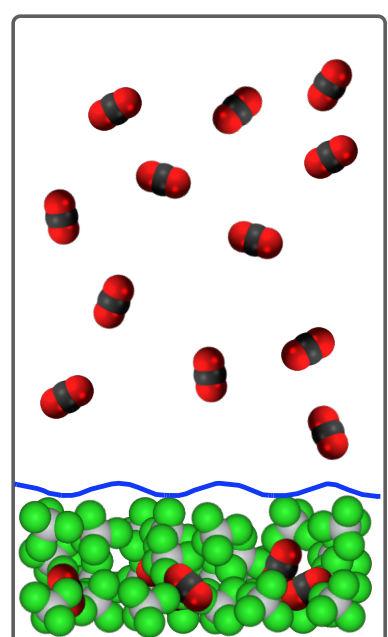


Recuperator Analysis:

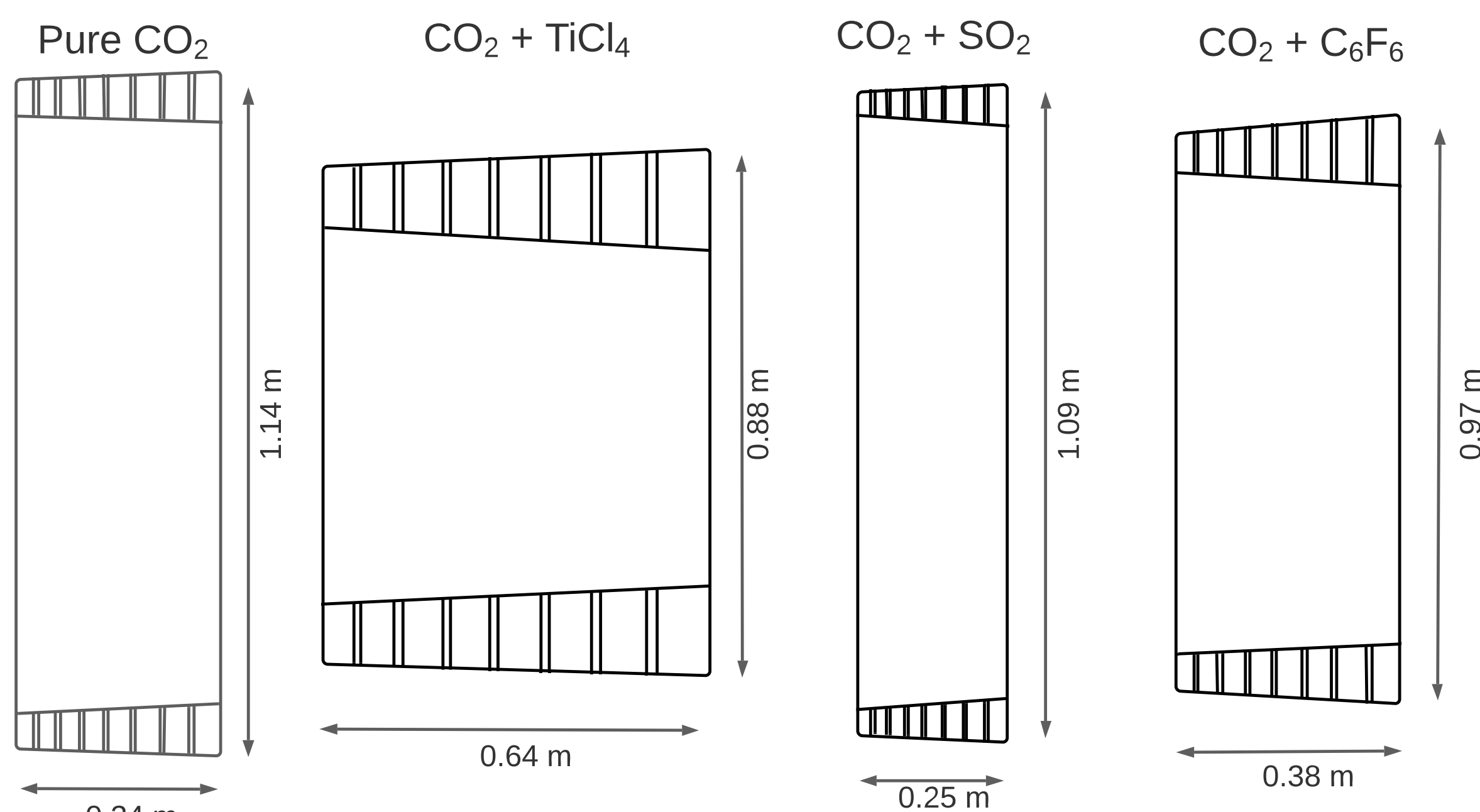
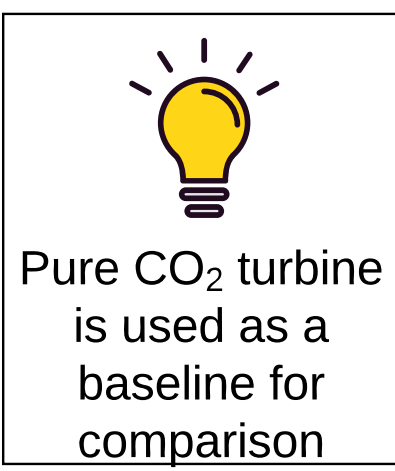
Recuperator pinch-point analysis showed that the choice of dopant affects the exergy destruction (irreversibility) during heat exchange. Molecularly complex dopants such as TiCl₄ and C₆F₆ reduce irreversibility and increases overall thermal efficiency.



However, the two heavy dopants completely condense whilst CO₂ remains largely in the gas phase - also known as 'fractionation'. This lowers the fluid's heat transfer coefficients and requires larger recuperators.



Turbine Analysis:



	Pure CO ₂	CO ₂ + TiCl ₄	CO ₂ + SO ₂	CO ₂ + C ₆ F ₆
Specific work	100%	-52%	-12%	-35%
Mass flow rate	100%	54%	-18%	17%
Volume flow rate	100%	-2%	-27%	-24%
Expansion ratio	100%	-24%	-2%	9%
Mach no.	100%	-14%	-1%	1%
Outlet temperature	100%	6%	0%	7%