Binary interaction parameter uncertainty in the optimisation of a transcritical cycle: consequences on cycle and turbine design

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Motivation

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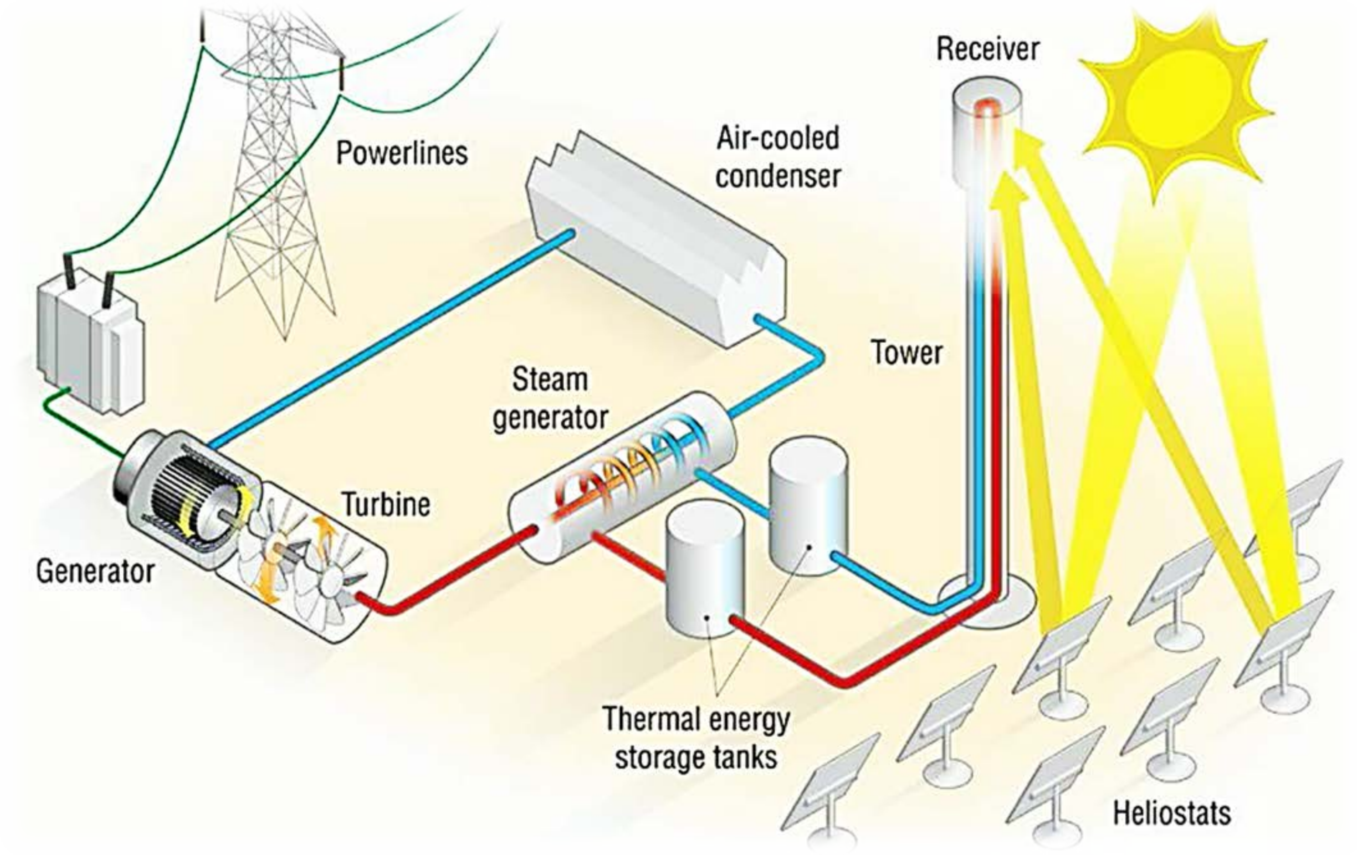
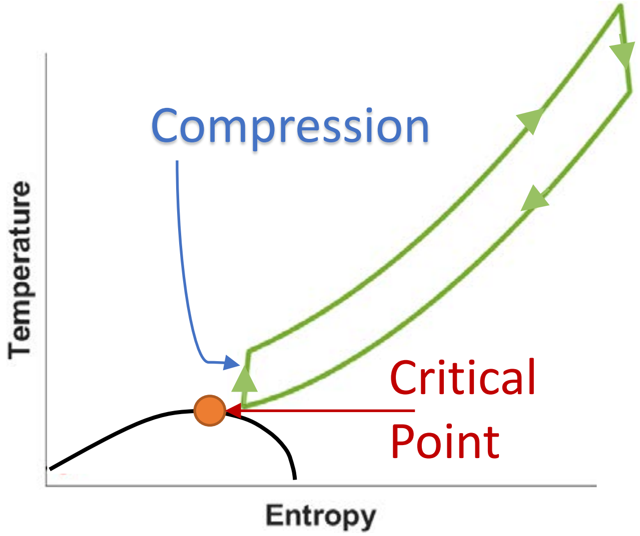
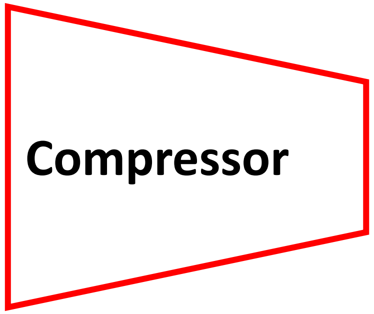
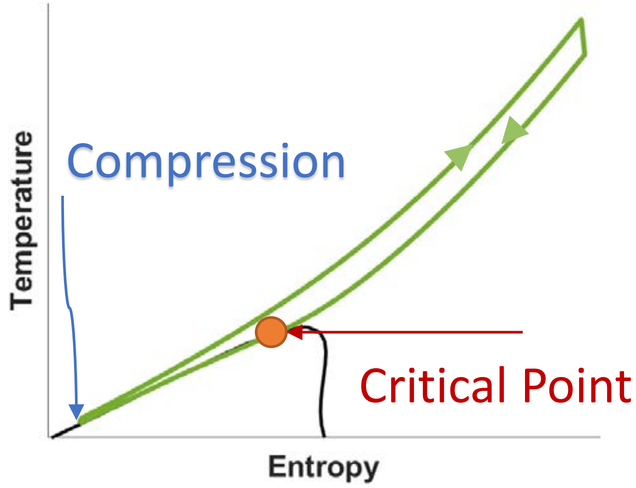
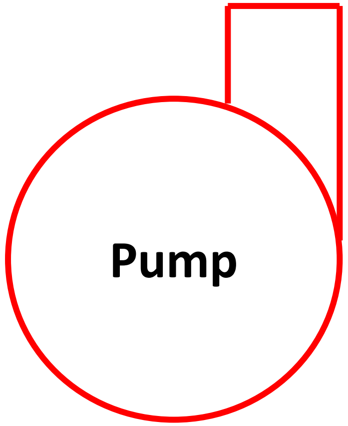
- The cost of Concentrated Solar Power (CSP) plants may be lowered by increasing power block efficiency, thus reducing solar field size
- The **SCARABEUS** project (H2020 funded) aims at developing CO_2 blends in CSP plants with maximum temperatures of 700°C, power block efficiency above 50% and cost of electricity below 96 €/MWh [2]
- CO_2 blends may achieve power block efficiencies above 50% by enabling condensation cycles



Typical Heliostat field connected to simple Rankine cycle through thermal energy storage tanks [1].

Motivation

	T-s Diagram	Compression Temp. & Press.	Compression phase and device
Brayton Cycle (pure CO_2)		$T > Critical\ Temperature$ $P > Critical\ Pressure$	Gas phase 
Rankine Cycle (CO_2 mixture)		$T < Critical\ Temperature$ $P < Critical\ Pressure$	Liquid phase  (Lower compression work)

Motivation

Selection of working fluid mixture → Setup of thermophysical property model → Process modelling

*For more details, please see:
G. Di Marcoberardino, C.M. Invernizzi, P. Iora, A. Ayub, D. Di Bona, P. Chiesa, M. Binotti, G. Manzolini,
Experimental and analytical procedure for the characterization of innovative working fluids for power plants applications,
Applied Thermal Engineering,
Volume 178,
2020,

Motivation

Selection of working fluid mixture

Setup of thermophysical property model

Process modelling

- ✓ Choice of Equation of State (EoS)
- ✓ Value of Binary Interaction Parameters (k_{ij})

} Uncertainty in estimated properties

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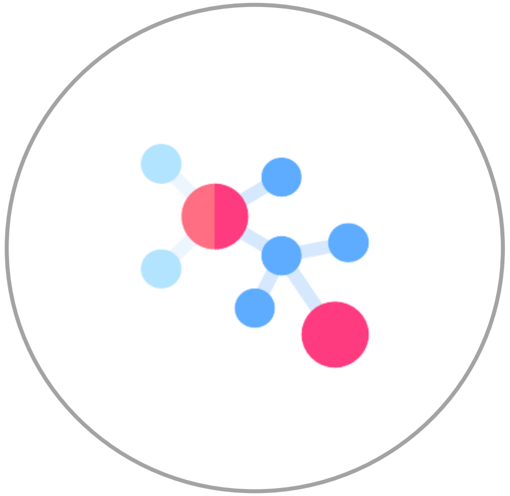
} Uncertainty in estimated properties → Uncertainty in process modelling

Methodology

Procedure:

1. Select Dopant (H_2S, NOD, C_6F_6)

(1)



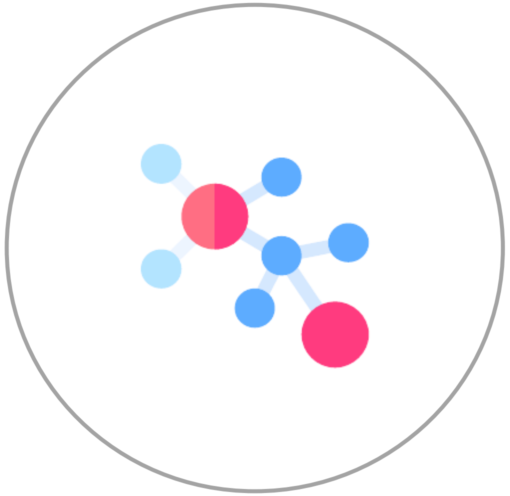
Methodology

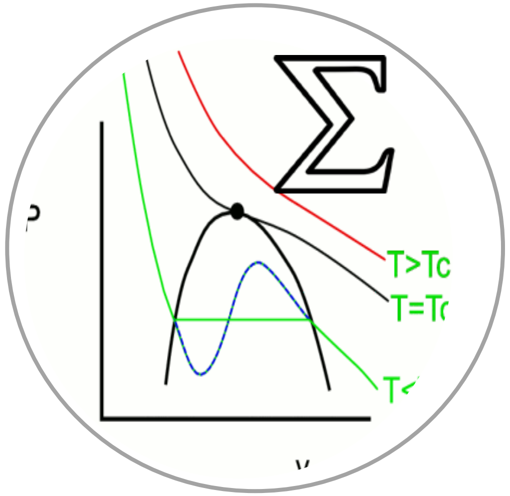
Procedure:

1. Select Dopant (H_2S, NOD, C_6F_6)

2. Select EoS (PR, BWRS, SRK, PC-SAFT)

(1)





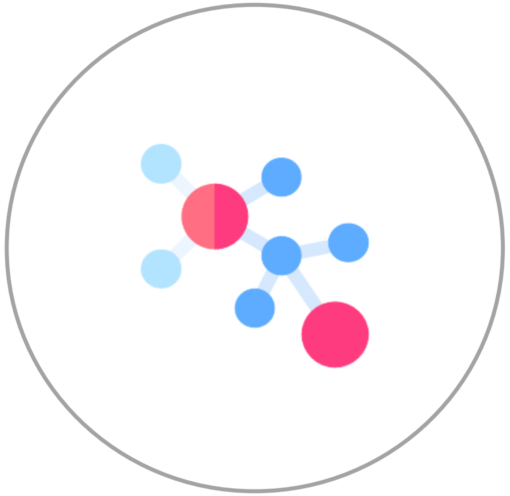
(2)

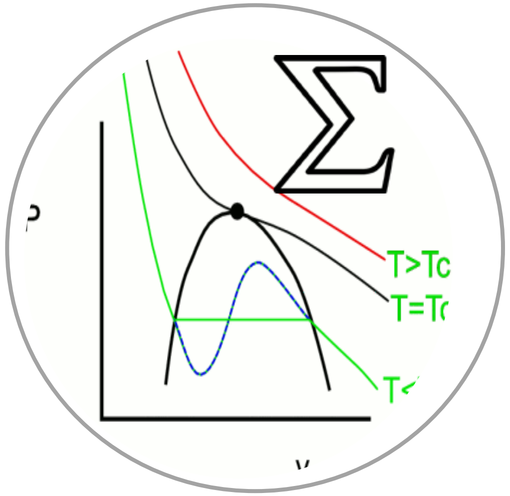
Methodology

Procedure:

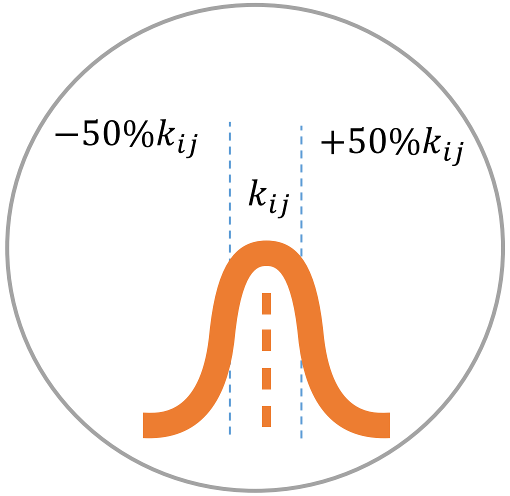
1. Select Dopant (H_2S, NOD, C_6F_6)
2. Select EoS (PR, BWRS, SRK, PC-SAFT)
3. Set binary interaction parameter

(1)





(2)



(3)

Methodology

Procedure:

1. Select Dopant (H_2S, NOD, C_6F_6)
2. Select EoS (PR, BWRS, SRK, PC-SAFT)
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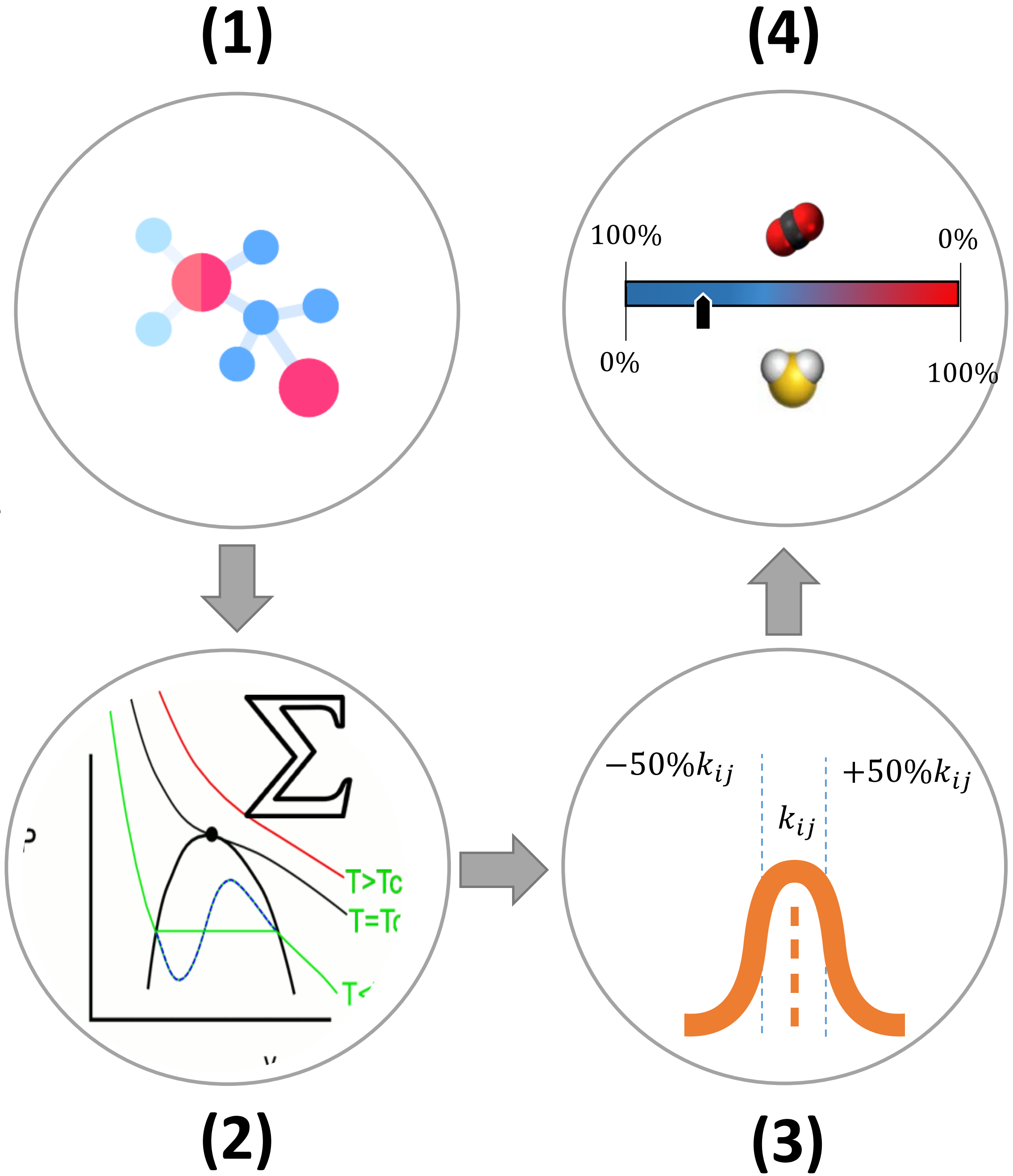
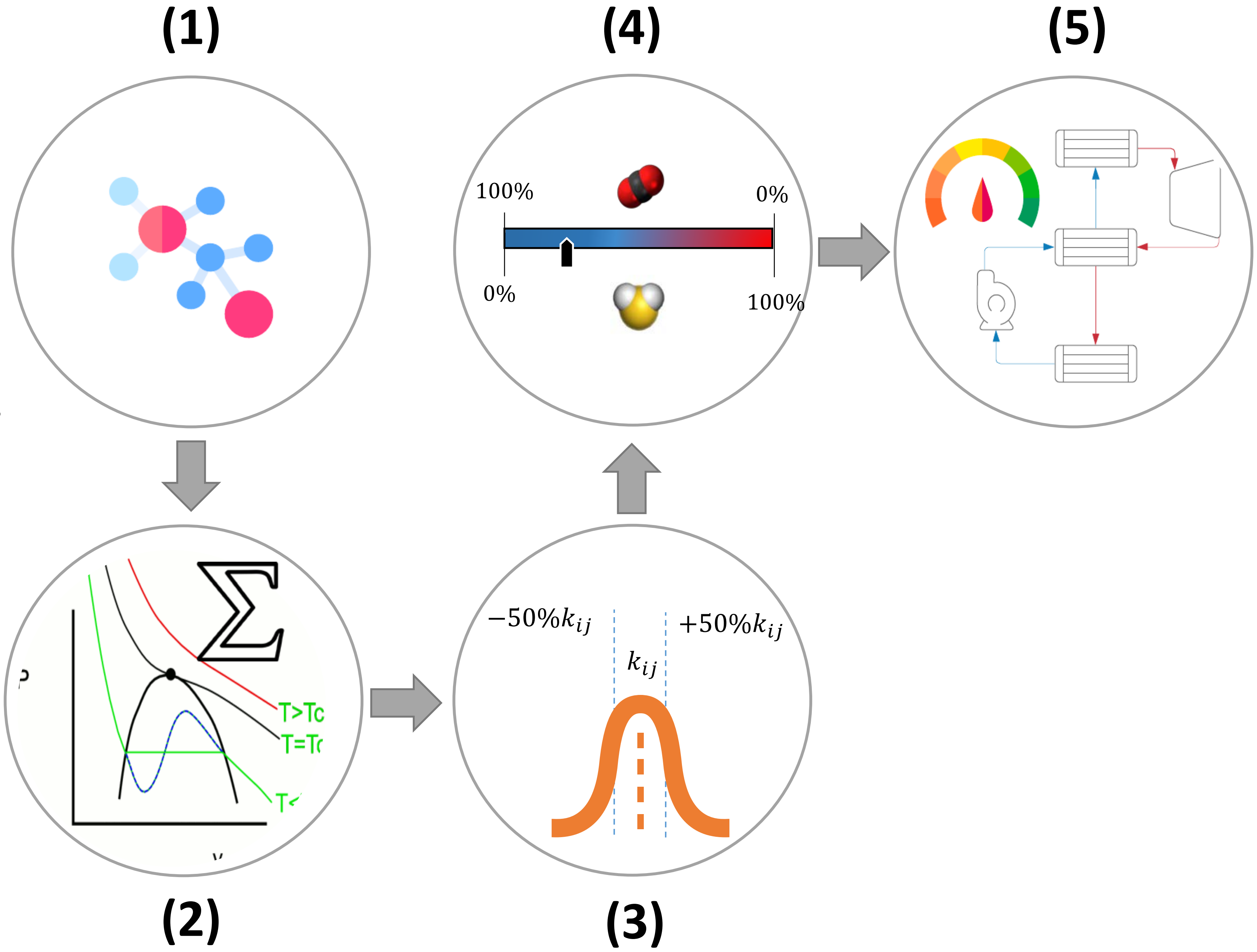
4. Set mixture composition



Methodology

Procedure:

1. Select Dopant (H_2S, NOD, C_6F_6)
2. Select EoS (PR, BWRS, SRK, PC-SAFT)
3. Set binary interaction parameter
4. Set mixture composition
5. Optimise cycle efficiency



Methodology

Procedure:

1. Select Dopant (H_2S, NOD, C_6F_6)
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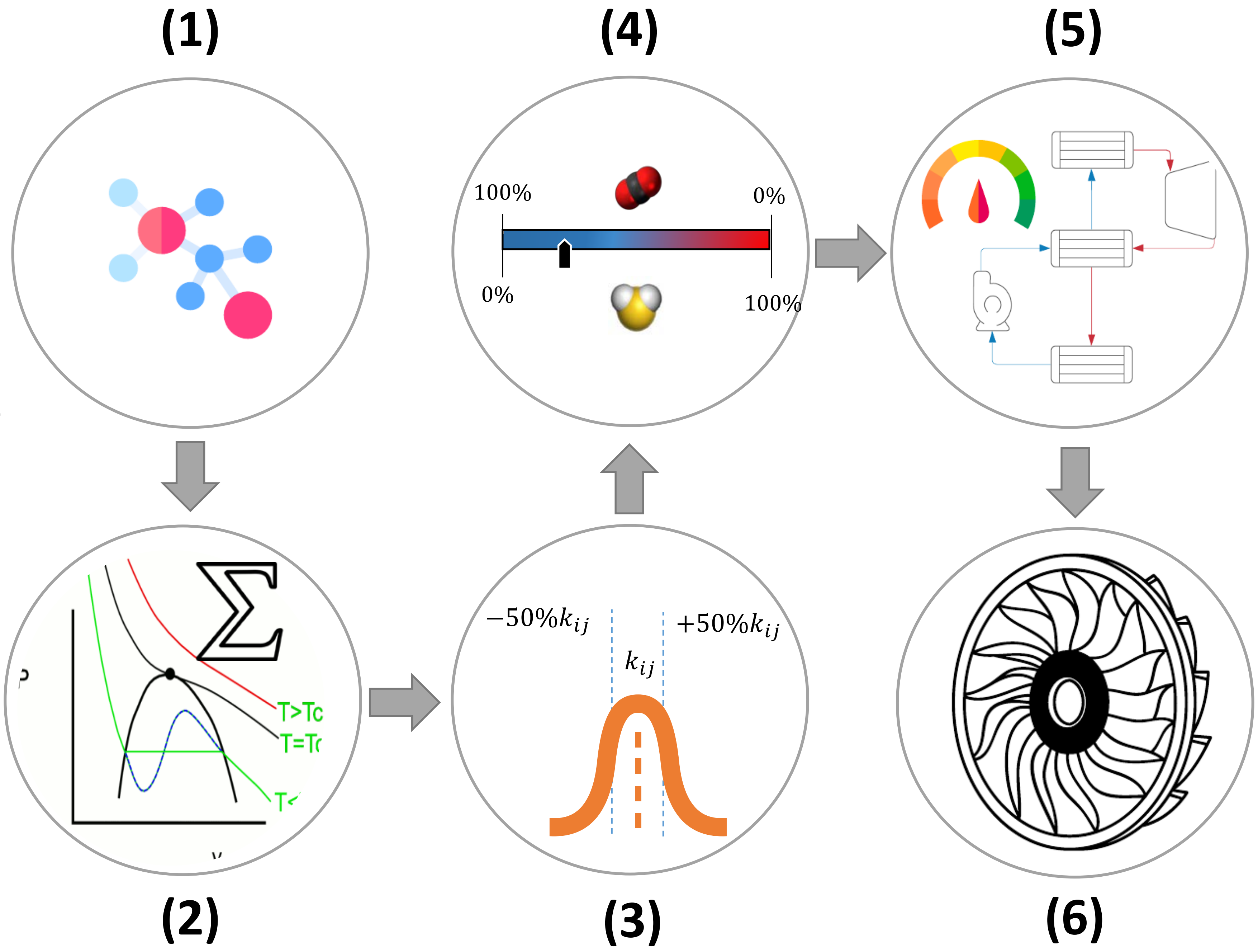
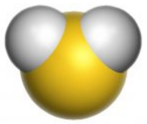
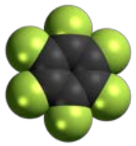
6. Generate turbine geometry

Steps 2 to 6 are repeated for each mixture

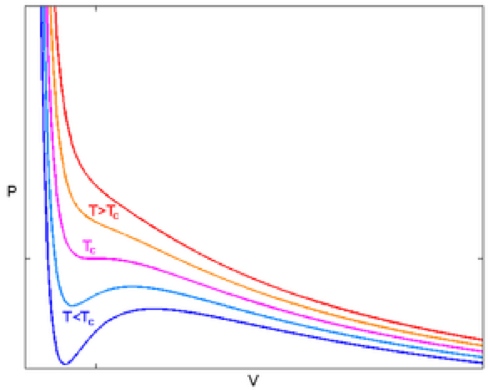


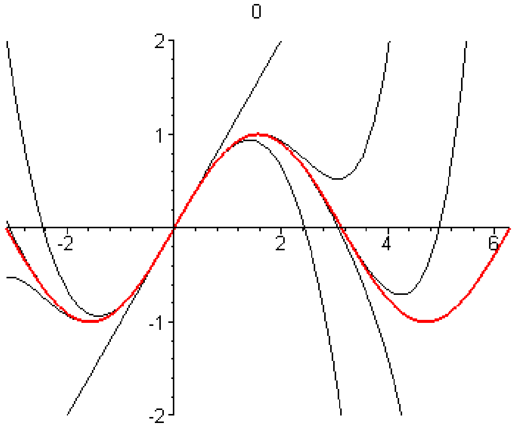
Dopants

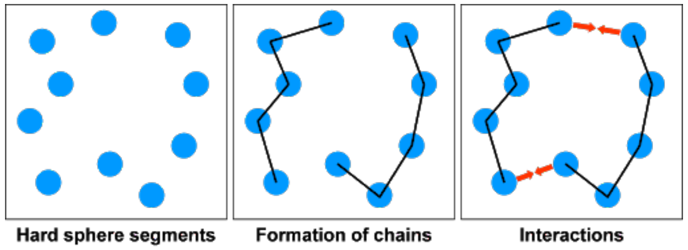
	Base Fluid	Dopants		
	Carbon Dioxide (CO_2)	Hydrogen Sulphide (H_2S)	Non-Organic Dopant (NOD)	Hexaflourobenzene (C_6F_6)
Molecular Shape				
Molecular Weight (g/mol)	**44.01**	**34.08**	**60<**	**186.1**
Critical Temperature (°C)	**31.10**	**100.4**	**150<**	**243.6**
Critical Pressure (bar)	**73.82**	**89.63**	**70<**	**32.73**

Equations of State (EoS)

- **EoS**
  - **Cubic**
    - **PR**
    - **SRK**
  - **Virial**
    - **BWRS**
  - **Helmholtz**
    - **PC-SAFT**







Tuning the binary interaction parameter (k_{ij})

Repeat to minimise error

k_{ij}

Set value of the binary interaction parameter

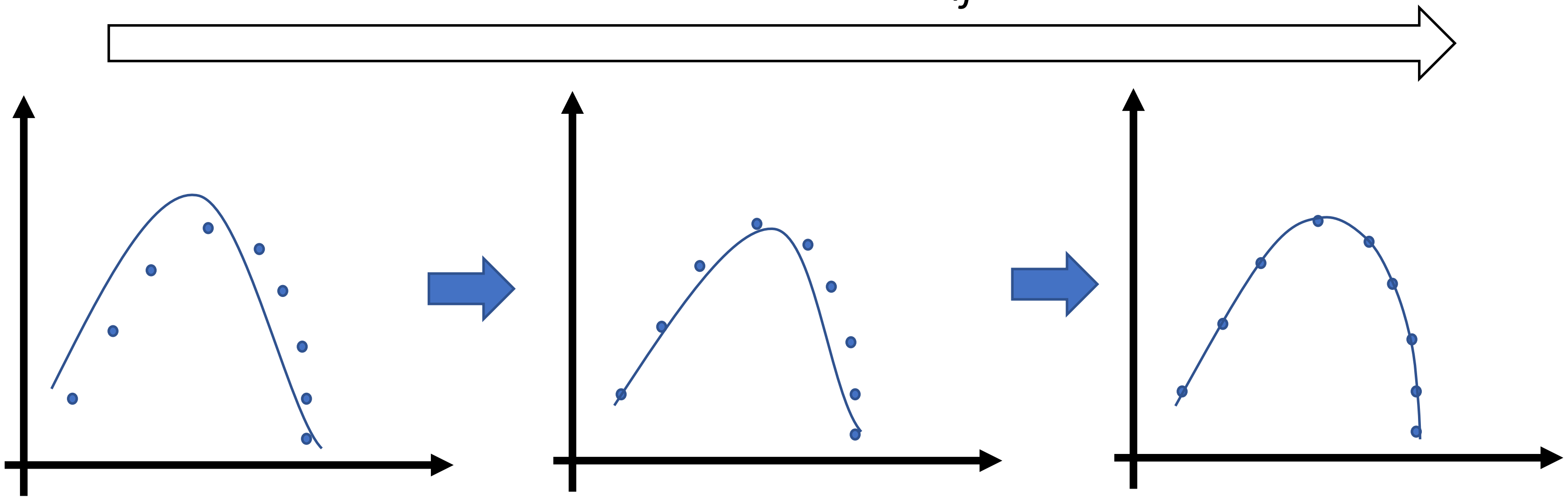
EoS

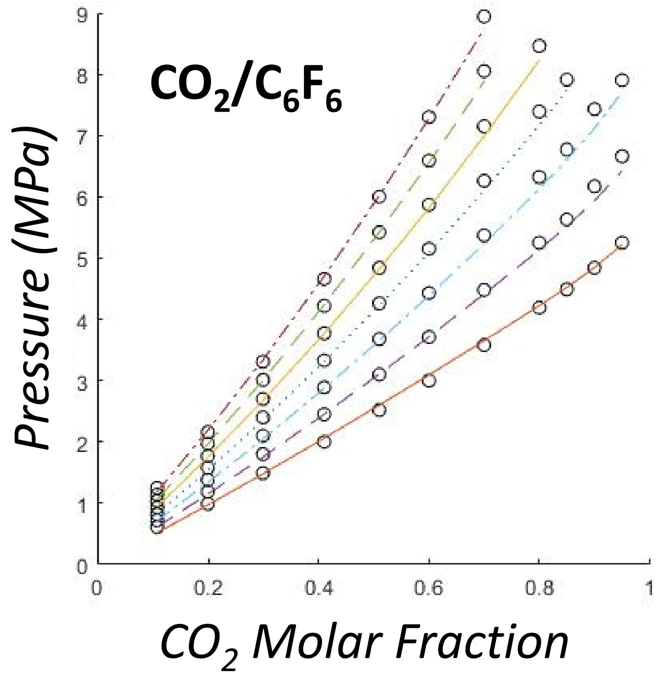
Calculate properties using the equation of state with calibrated k_{ij}

Error

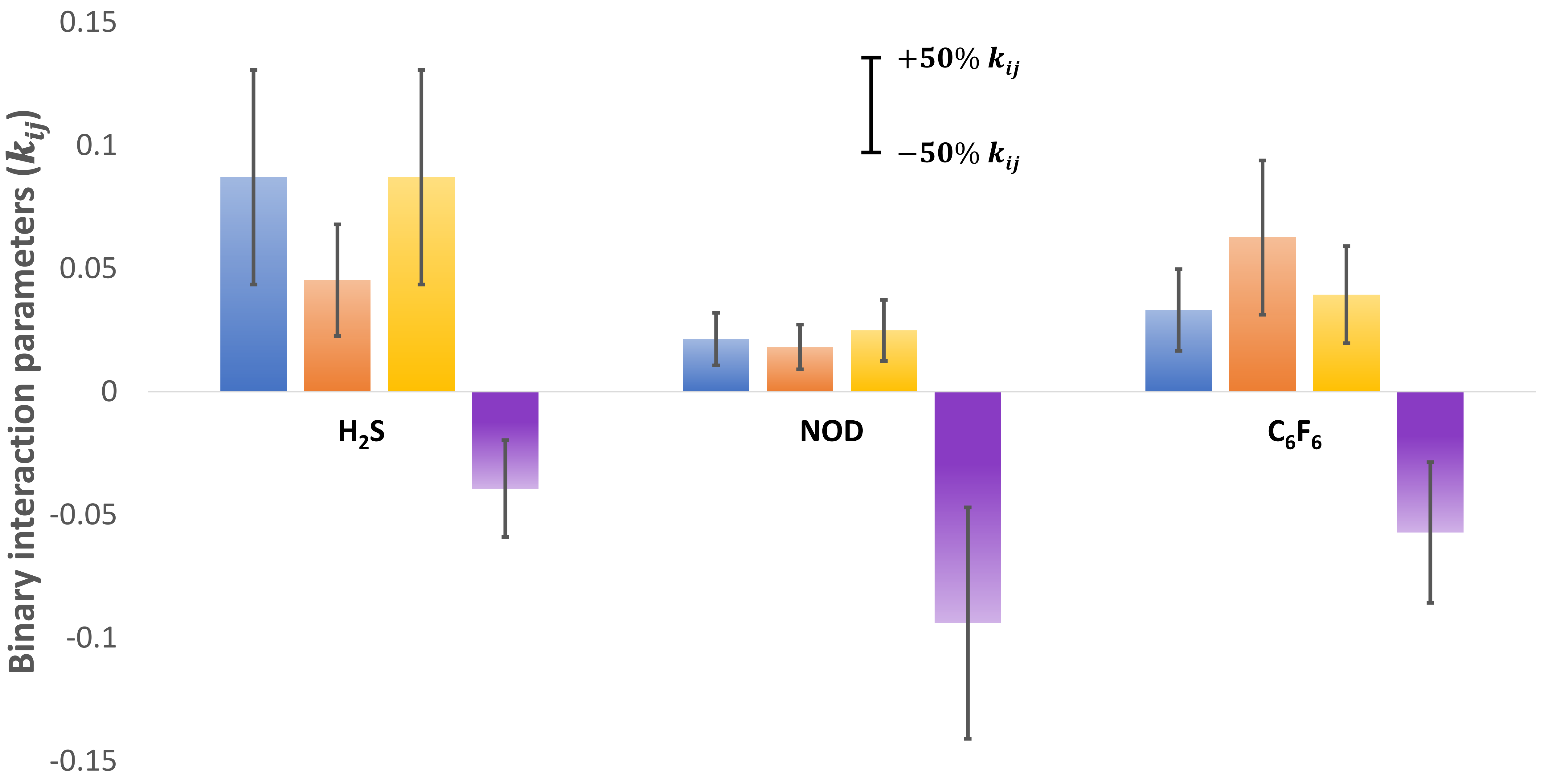
Compute error between the experimental and calculated properties.

Calibration of k_{ij}





Variation in the binary interaction parameters (k_{ij})



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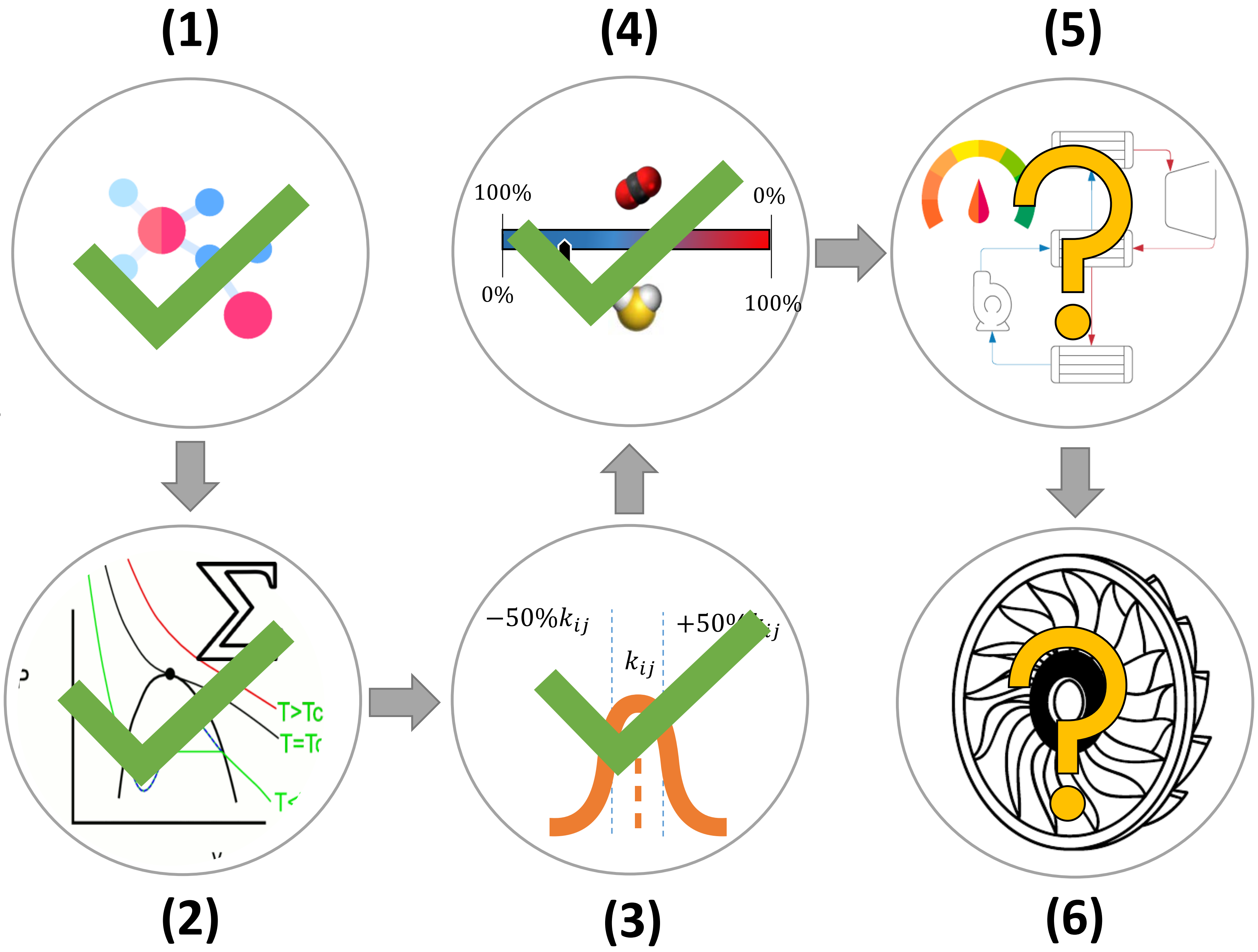
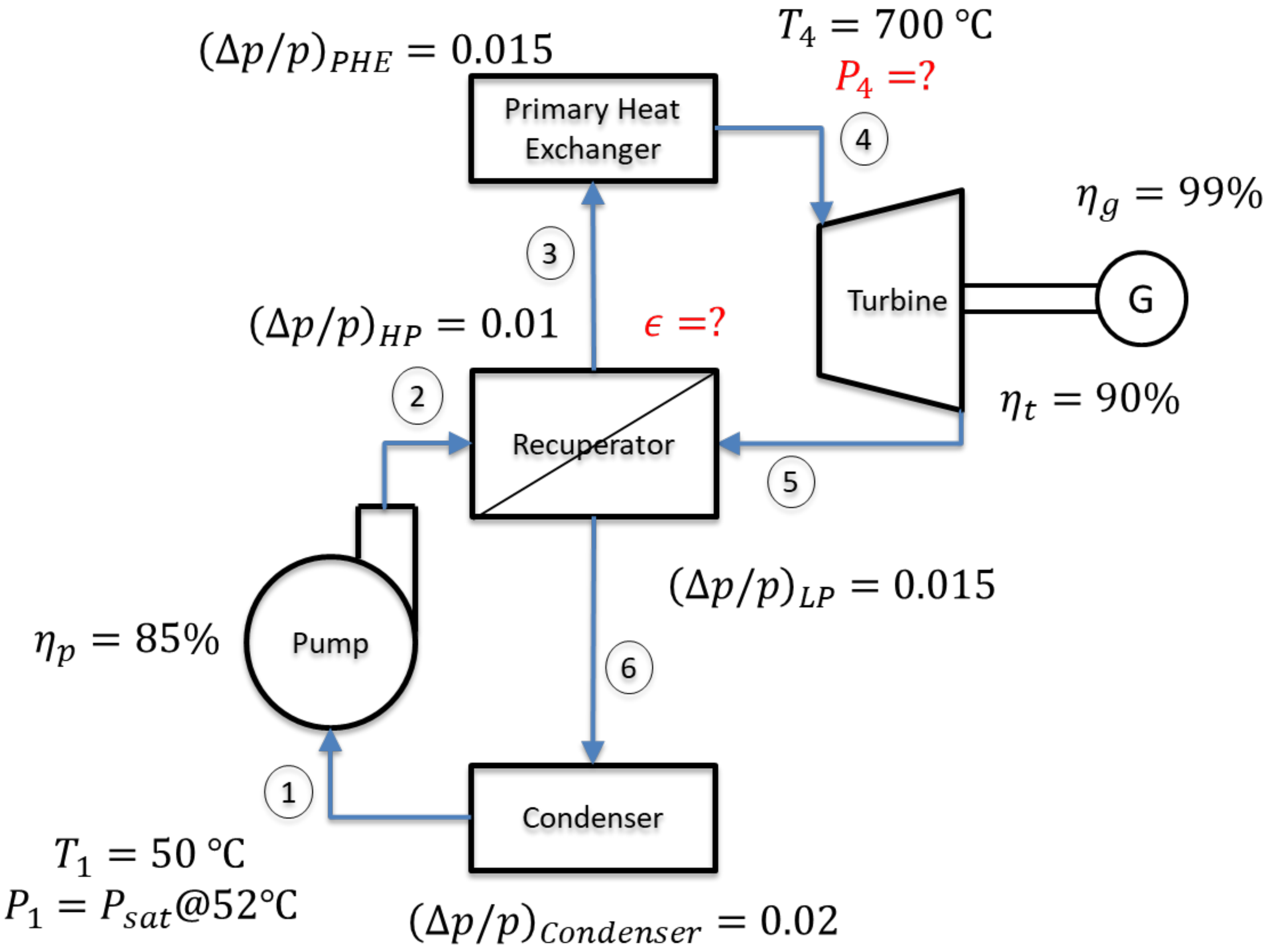


Cycle assumptions:

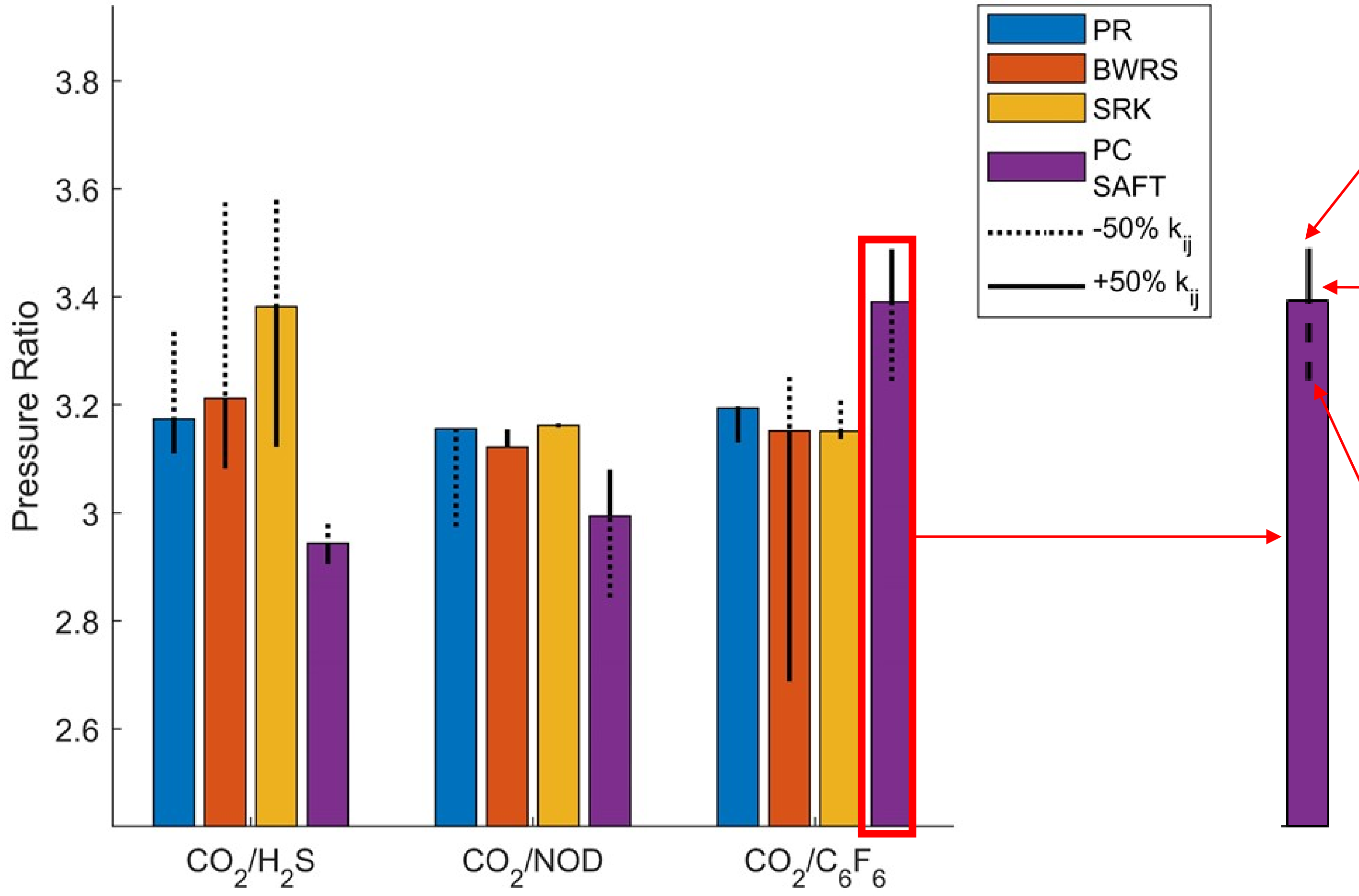
- 100 MW_e plant capacity
- Minimum Internal Temperature Approach (MITA) of 5 °C in recuperator
- Pump inlet pressure is chosen based on 2 °C subcooling in the condenser

Turbine Design Parameter	Value
Rotational speed (RPM)	3000
Number of stages (%)	4
Turbine efficiency (η_t)	90
Loading coefficient (ψ)	1.65
Flow coefficient (ϕ)	0.23
Degree of reaction (Λ)	0.5



Results

Legend overview



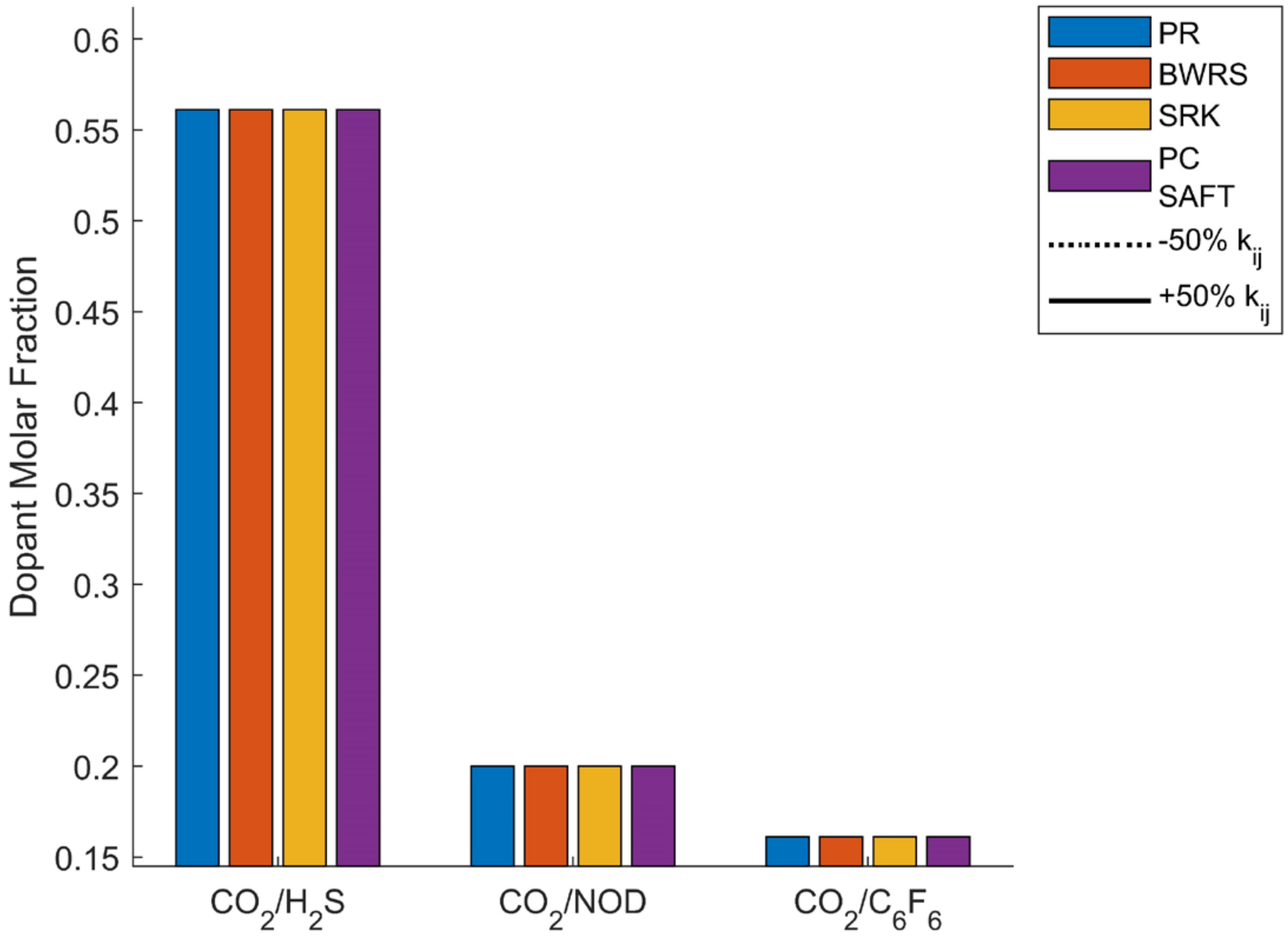
$CO_2/C_6F_6 + PC-SAFT + 1.5\ k_{ij}$

$CO_2/C_6F_6 + PC-SAFT + 1.0\ k_{ij}$

$CO_2/C_6F_6 + PC-SAFT + 0.5\ k_{ij}$

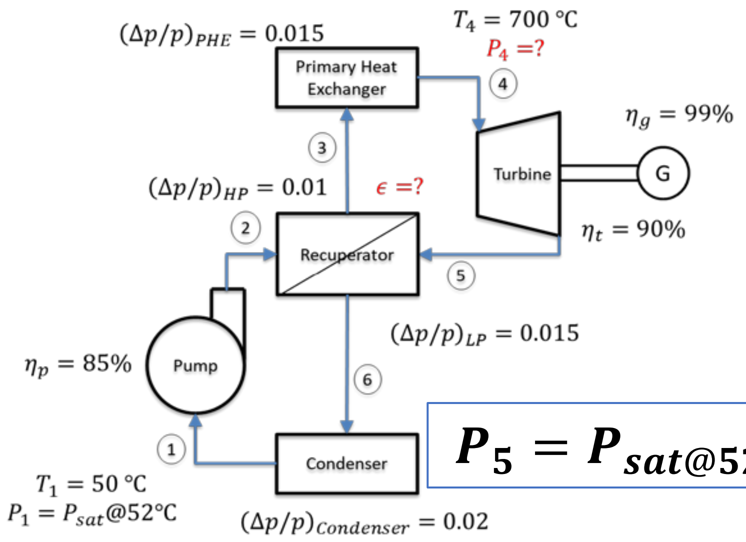
Optimal dopant fraction

- Neither the choice of the EoS nor the variation in k_{ij} effect the choice of the optimal dopant fraction which maximises efficiency.
- In other words, the same mixture composition will be chosen regardless of the thermophysical property model being used.

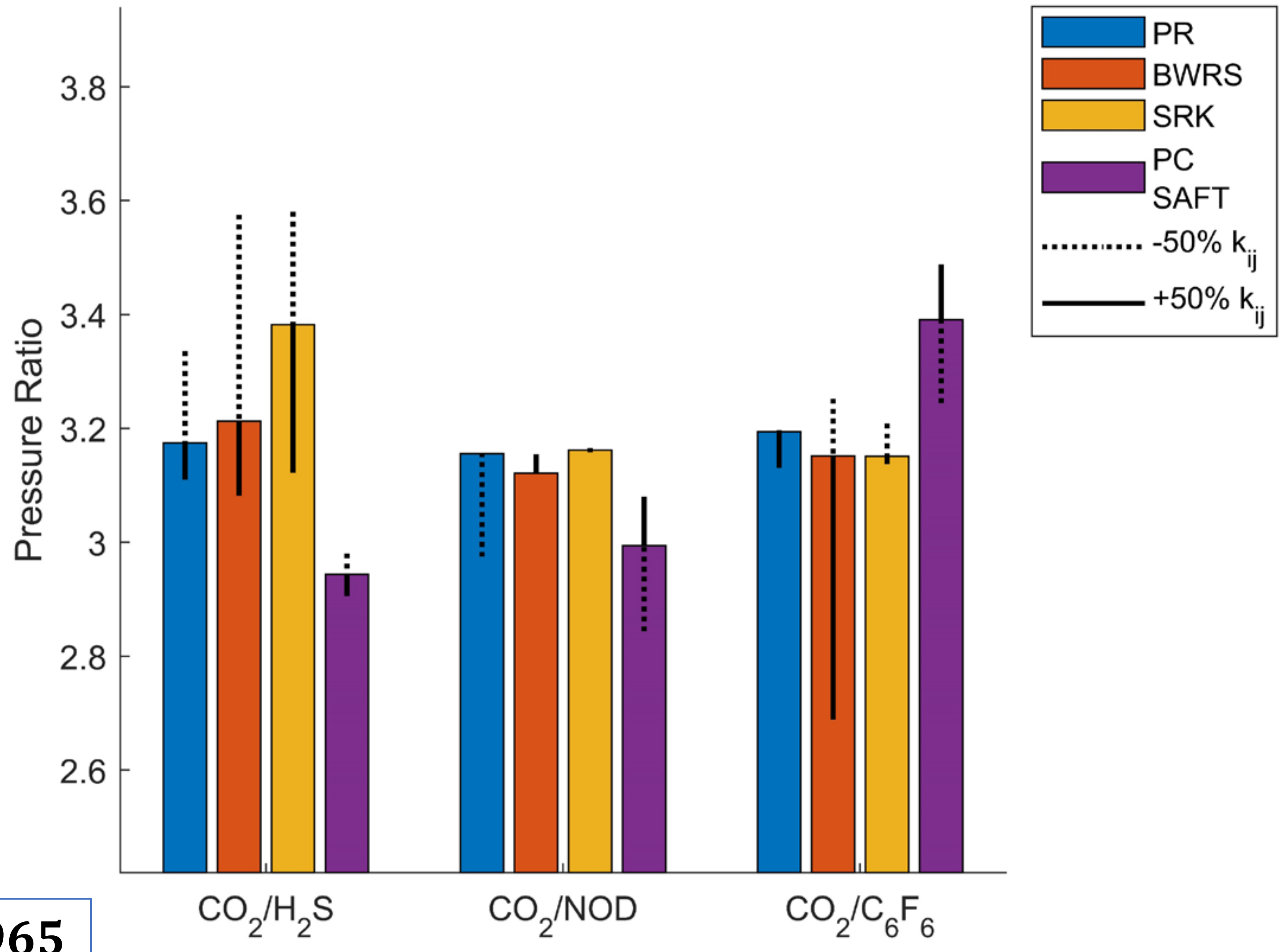


Pressure ratio

- The pressure ratio corresponding to the optimal cycle conditions varies with the fluid model.
- Since the cycle max pressure is uniform for all cycles (250 bar), then the change in pressure ratio is a direct consequence of the calculated pump inlet pressure ($P_1 = P_{sat@52℃}$).

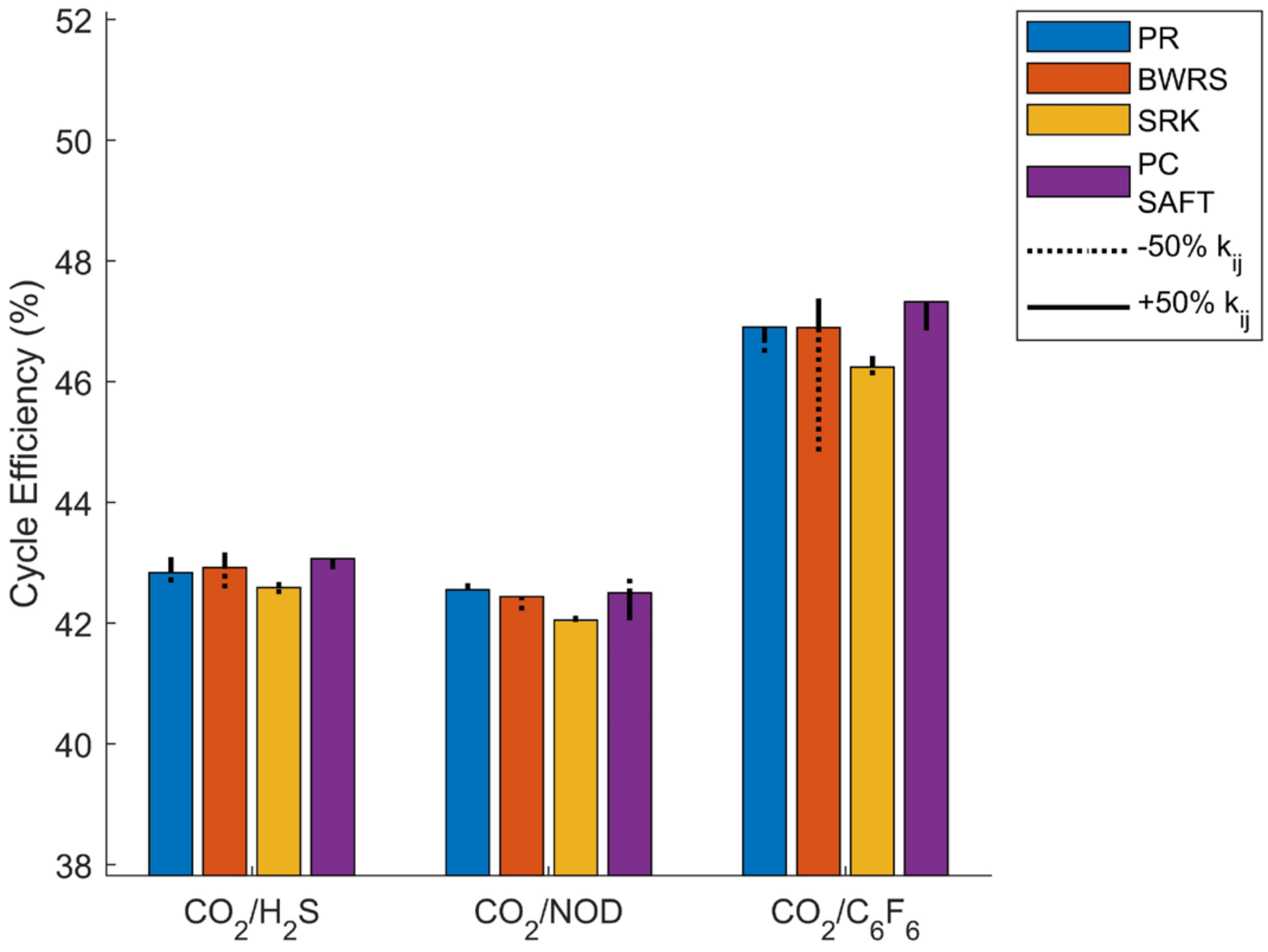


$$P_5 = P_{sat@52℃}/0.965$$



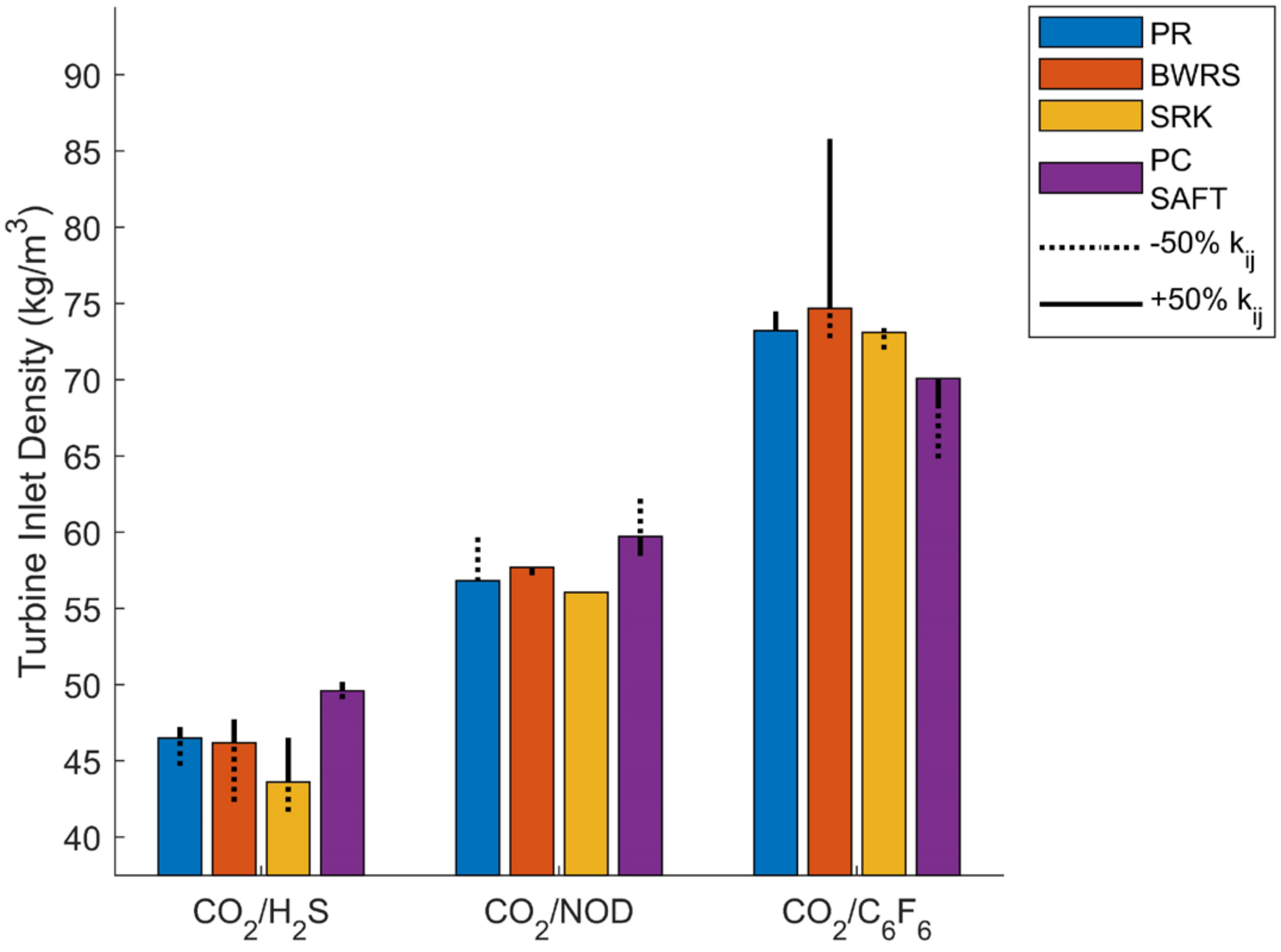
Thermal efficiency

- Thermal efficiency is affected by the EoS and the value of kij, but this effect differs depending on the mixture.
- 1% difference between SRK and PC-SAFT for CO_2/C_6F_6.
- Less than 0.5% difference between the EoS of CO_2/H_2S and CO_2/NOD.
- More than 2% drop in efficiency with -50% variation in kij when modelling CO_2/C_6F_6 using BWRS.



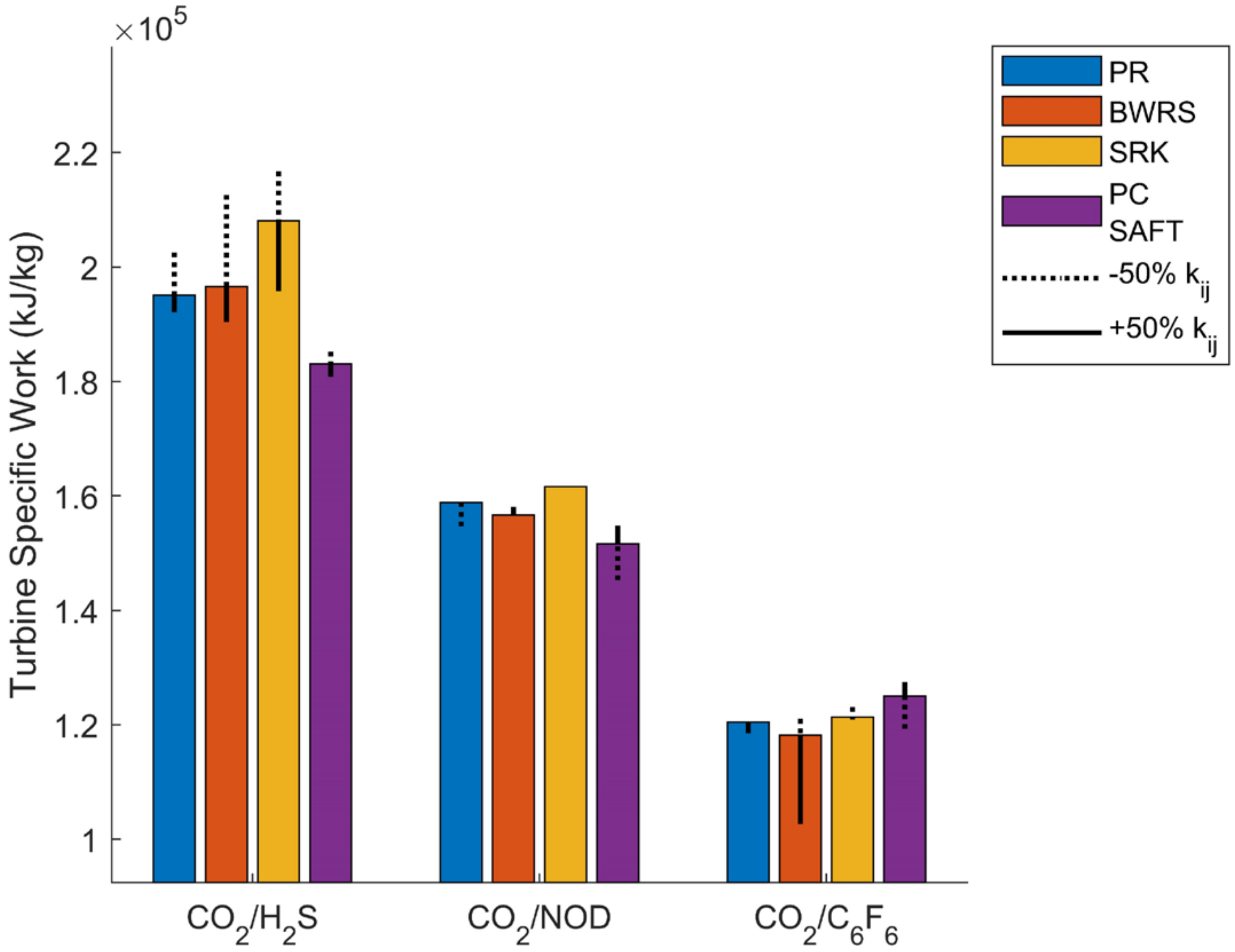
Turbine Inlet Density

- CO_2/H_2S is affected the most by the choice of the EoS (SRK vs PC-SAFT).
- The cubic EoS (PR and SRK) and PC-SAFT are generally less sensitive to kij than BWRS.
- BWRS is affected the most by kij variation, especially for CO_2/C_6F_6, therefore precise kij values are recommended when employing the BWRS EoS.



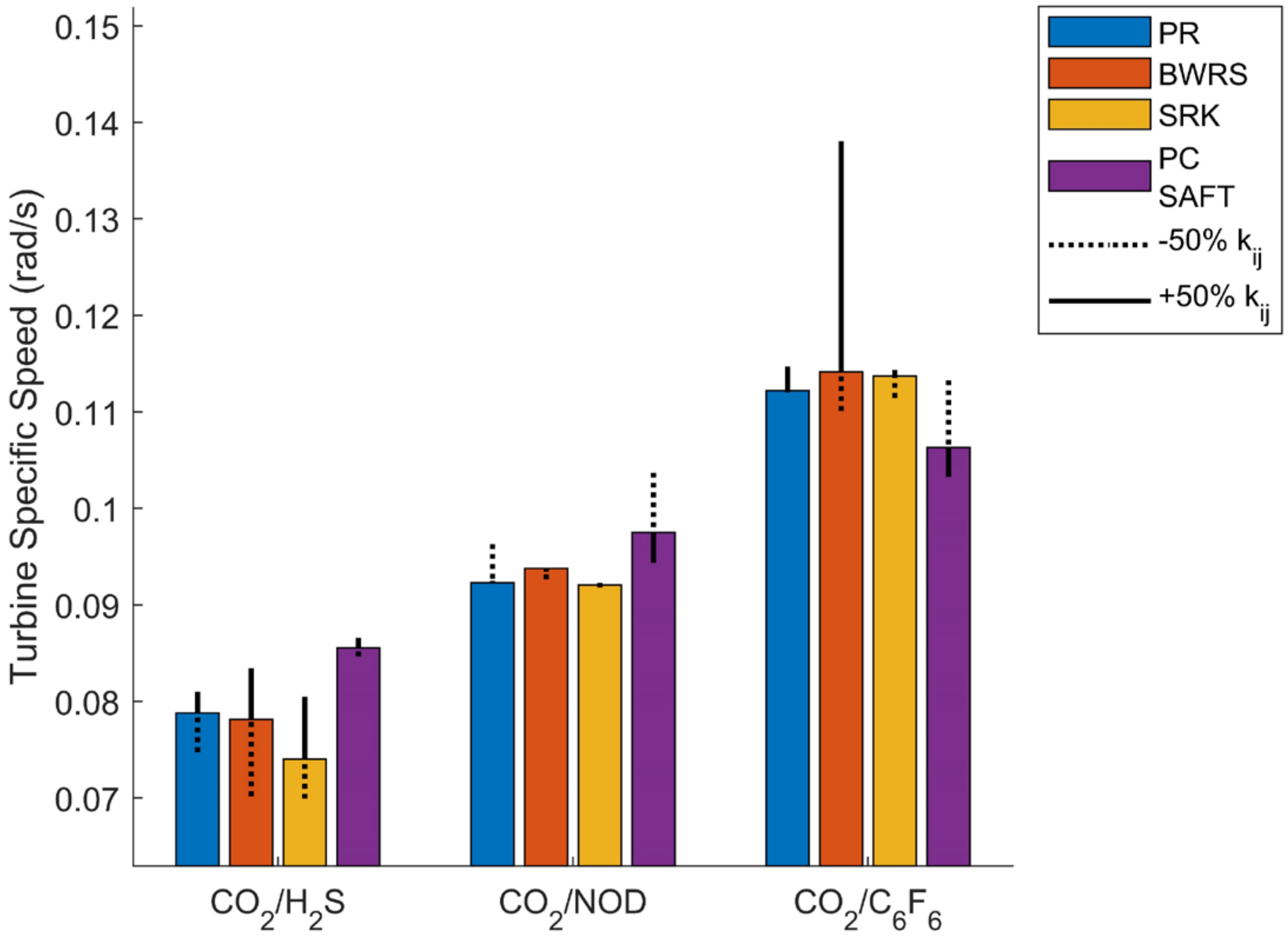
Turbine Specific Work

- Simpler working fluid mixtures have higher specific work.
- Specific work may affect turbine geometry for a set of fixed design parameters.
- 13.7% difference observed between SRK and PC-SAFT for CO_2/H_2S could produce slightly different turbine designs, as seen later.

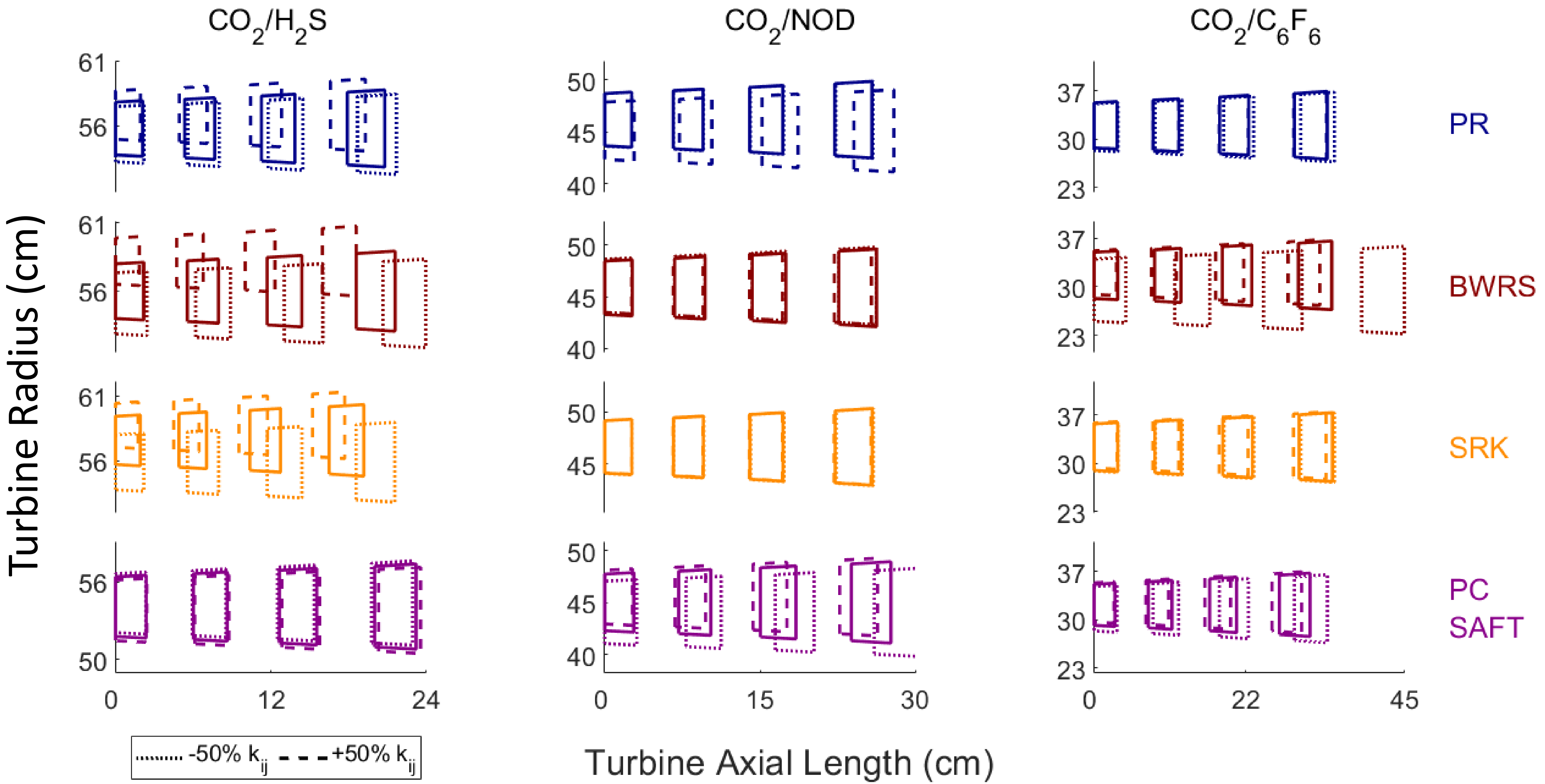


Specific Speed

- Calculated at exit conditions.
- Indication of turbine shape and size.
- 21% difference due to +50% increase in kij for BWRS of CO_2/C_6F_6. But only 0.2 rad/s change.



Rotor Blade Geometry



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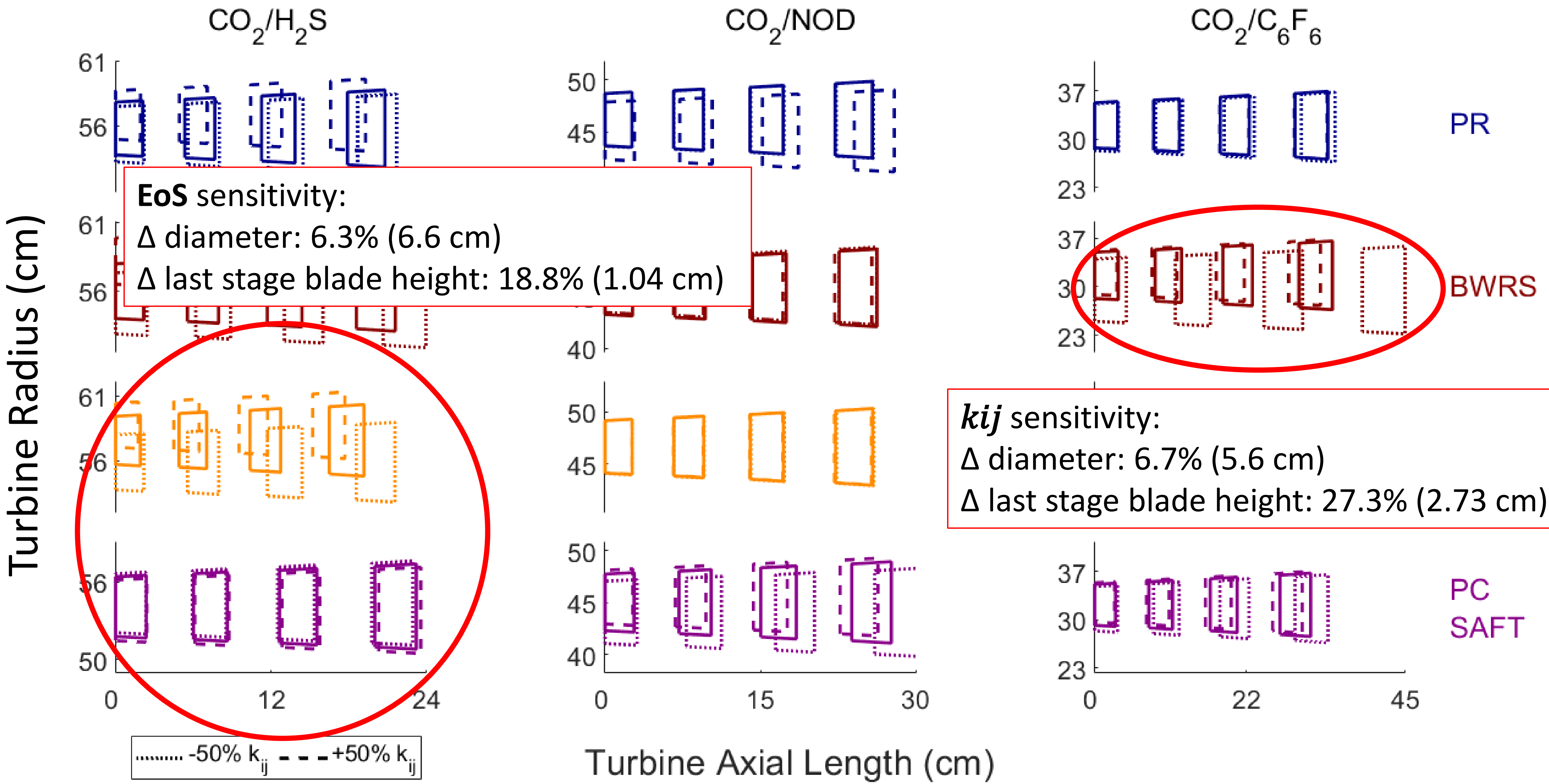
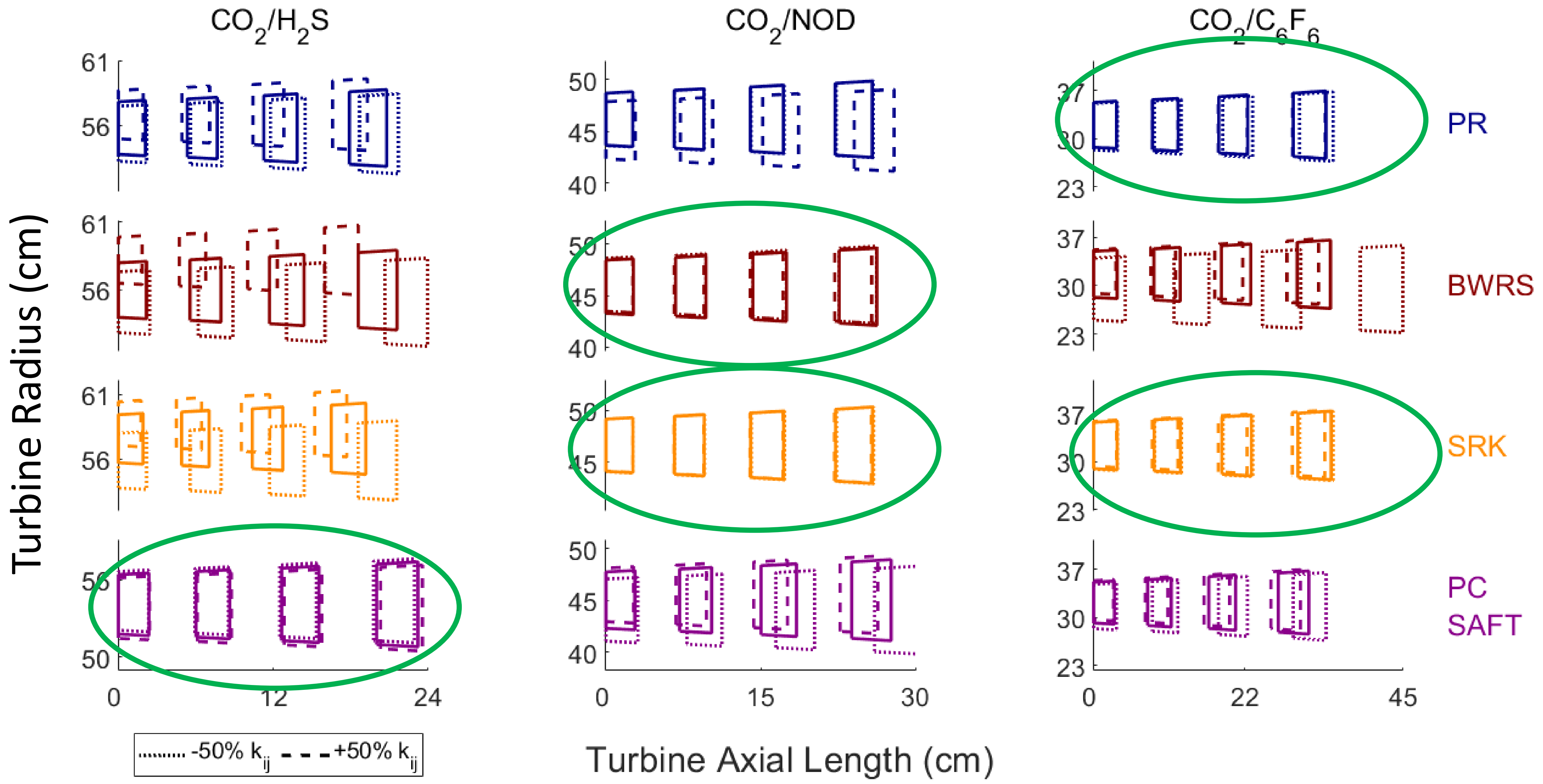


EoS sensitivity:
Δ diameter: 6.3% (6.6 cm)
Δ last stage blade height: 18.8% (1.04 cm)

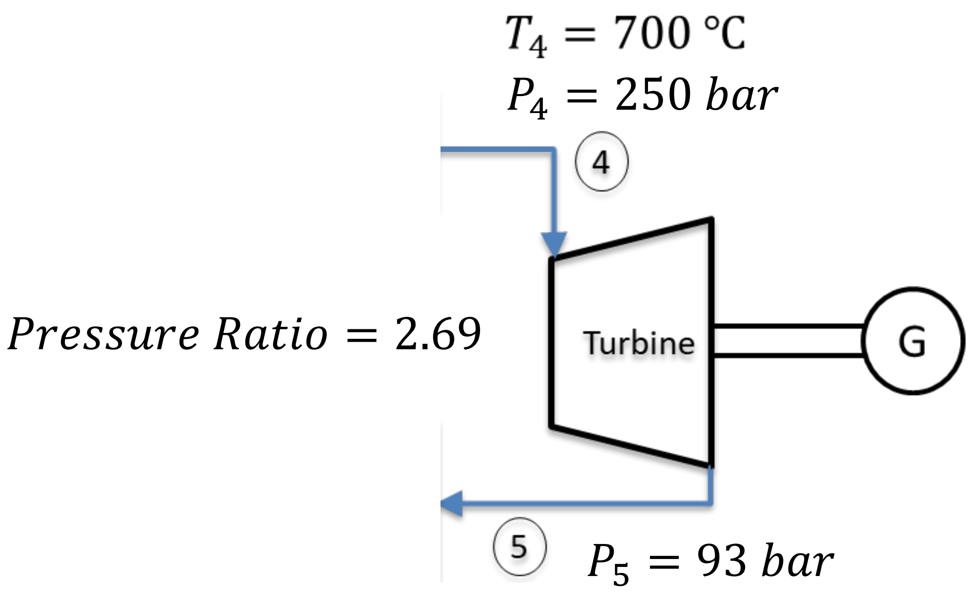
kij sensitivity:
Δ diameter: 6.7% (5.6 cm)
Δ last stage blade height: 27.3% (2.73 cm)

Rotor Blade Geometry

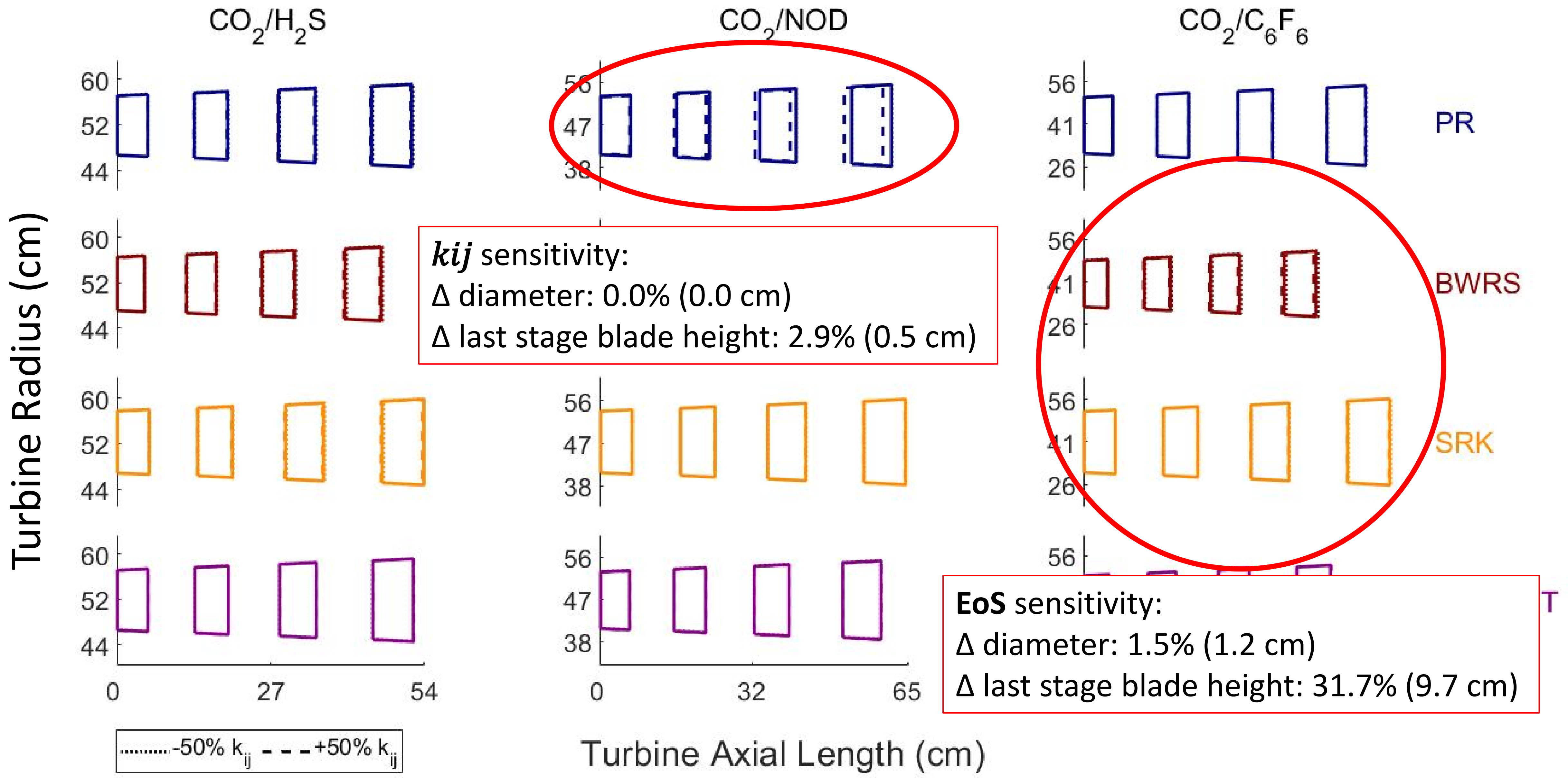


Fixed turbine model assumptions:

- Detachment of turbine from varying cycle conditions.
- Fixed turbine back pressure for all fluid models
- Fixed pressure ratio.



Rotor blade geometry for fixed back pressure



kij sensitivity:
Δ diameter: 0.0% (0.0 cm)
Δ last stage blade height: 2.9% (0.5 cm)

EoS sensitivity:
Δ diameter: 1.5% (1.2 cm)
Δ last stage blade height: 31.7% (9.7 cm)

Conclusion and future work

- Sensitivity to the fluid model depends on the mixture being used.
- Avoid BWRS in the absence of experimental data.
- It is recommended to use either the cubic or PC SAFT EoS as they are the least sensitive to the interaction parameter uncertainty
- CO_2/H_2S showed the highest sensitivity to the fluid model.
- Recommended to account for turbine aerodynamic losses.
- Most of the interaction parameter sensitivity stems from the variation in turbine back pressure.

Acknowledgement

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Thank You!

References

1. Praveen, R., Performance analysis and optimization of central receiver solar thermal power plants for utility scale power generation. Sustainability, 2020. 12(1): p. 127.
2. M. Binotti, G. Di Marcoberardino, P. Iora, and C. Invernizzi, “SCARABEUS : Supercritical carbon dioxide / alternative fluid blends for efficiency upgrade of solar power plants SCARABEUS : Supercritical Carbon Dioxide / Alternative Fluid Blends for Efficiency Upgrade of Solar Power Plants,” vol. 130002, no. December, 2020.