Photo by Stefan Els

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Recommended for you:
What chemical engineering can learn from Netflix

Dr Jamie Cripwell

2024 Stellenbosch Engineering Industry Showcase

The Netflix Prize

The Netflix Prize

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The Netflix Prize

The Netflix Prize

$\equiv$

$$\boldsymbol{R} \in (m \times n)$$

$\times$

The Netflix Prize

n movies

m users

4	2	1	5		
1		5		3	
	5		4		2
		4			

$\equiv$

$$\boldsymbol{R} \in (m \times n)$$

$\times$

$r_{ij} \ni$ rating of user i for movie j

The Netflix Prize

n movies

m users

4	2	1	5		
1		5		3	
	5		4		2
		4			

$\equiv$

$\boldsymbol{U} \in (m \times k)$

$\boldsymbol{V}^{\boldsymbol{T}} \in (k \times n)$

$$\boldsymbol{R} = \boldsymbol{U}\boldsymbol{V}^{\boldsymbol{T}}$$

The Netflix Prize

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n movies

m users

4	2	1	5		
1		5		3	
	5		4		2
		4			

$\equiv$

m users

$U \in (m \times k)$

n movies

$V^T \in (k \times n)$

$$R = UV^T$$

$k \equiv latent\ features$

The Netflix Prize

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“Matrix Completion”

n movies

m users

4	2	1	5	2	3
1	3	5	4	3	5
3	5	2	4	3	2
1	4	4	1	3	5

$\equiv$

n movies

m users

$\boldsymbol{U} \in (m \times k)$

$\boldsymbol{V}^{\boldsymbol{T}} \in (k \times n)$

$$\boldsymbol{R} = \boldsymbol{U}\boldsymbol{V}^{\boldsymbol{T}}$$

$k \equiv latent\ features$

The Netflix Prize

"Matrix Completion"

n movies

m users

4	2	1	5	2	3
1	3	5	4	3	5
3	5	2	4	3	2
1	4	4	1	3	5

$\equiv$

m users

$\boldsymbol{U} \in (m \times k)$

n movies

$\boldsymbol{V}^{\boldsymbol{T}} \in (k \times n)$

$$\boldsymbol{R} = \boldsymbol{U}\boldsymbol{V}^{\boldsymbol{T}}$$

$$\underbrace{k \equiv latent\ features}$$

"Collaborative Filtering"

Relevance to Chemical Engineering?

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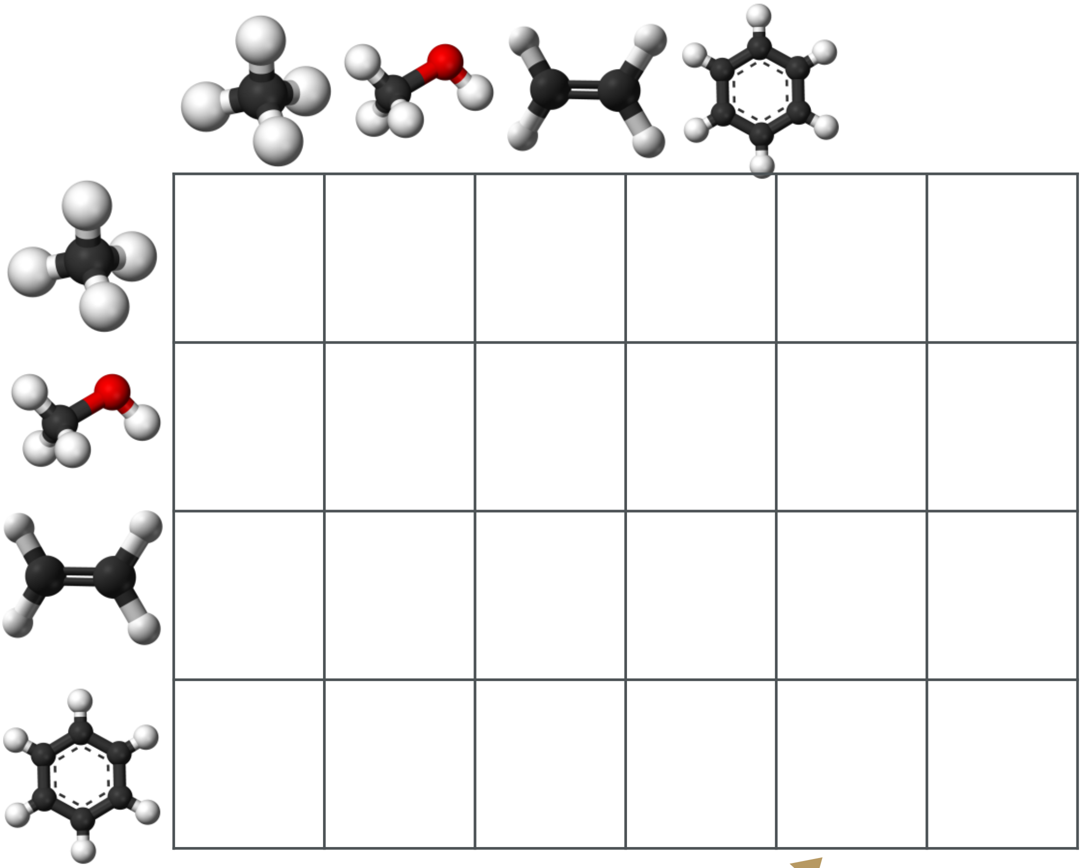
"Matrix Completion"



n species

$\equiv$ m species

$\boldsymbol{U} \in (m \times k)$

$\boldsymbol{V}^{\boldsymbol{T}} \in (k \times n)$

$\boldsymbol{R} = \boldsymbol{U}\boldsymbol{V}^{\boldsymbol{T}}$

$\underbrace{k \equiv latent\ features}$

"Collaborative Filtering"

Relevance to Chemical Engineering?

$$\begin{array}{cc} & n\ \text{species} \\ m\ \text{species} & \begin{bmatrix} d_{11} & \cdots & \cdots & d_{14} \\ \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ d_{41} & \cdots & \cdots & d_{44} \end{bmatrix} \end{array}$$

$\boldsymbol{D} \ni$ mixture property data

Relevance to Chemical Engineering?

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$$\begin{array}{cc} & n \text{ species} \\ m \text{ species} & \begin{bmatrix} d_{11} & \cdots & \cdots & d_{14} \\ \vdots & \ddots & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ d_{41} & \cdots & \cdots & d_{44} \end{bmatrix} \end{array}$$

$\boldsymbol{D} \ni$ mixture property data

$\boldsymbol{d}_{ii} \ni$ pure component

$\boldsymbol{d}_{ij} \ni$ binary mixture

Success stories…

- Compared to UNIFAC Dortmund: "…error is below 0.1 for 37.4% of the predictions with UNIFAC, whereas the proposed MCM achieves the same accuracy for 50.0% of the predictions."

n solutes

m solvents

$$\begin{bmatrix} d_{11} & \cdots & \cdots & d_{14} \\ \vdots & & & \vdots \\ \vdots & & & \vdots \\ d_{41} & \cdots & \cdots & d_{44} \end{bmatrix}$$

γ_{ij}^{∞}

240 solutes
250 solvents

$\equiv$

m solvents

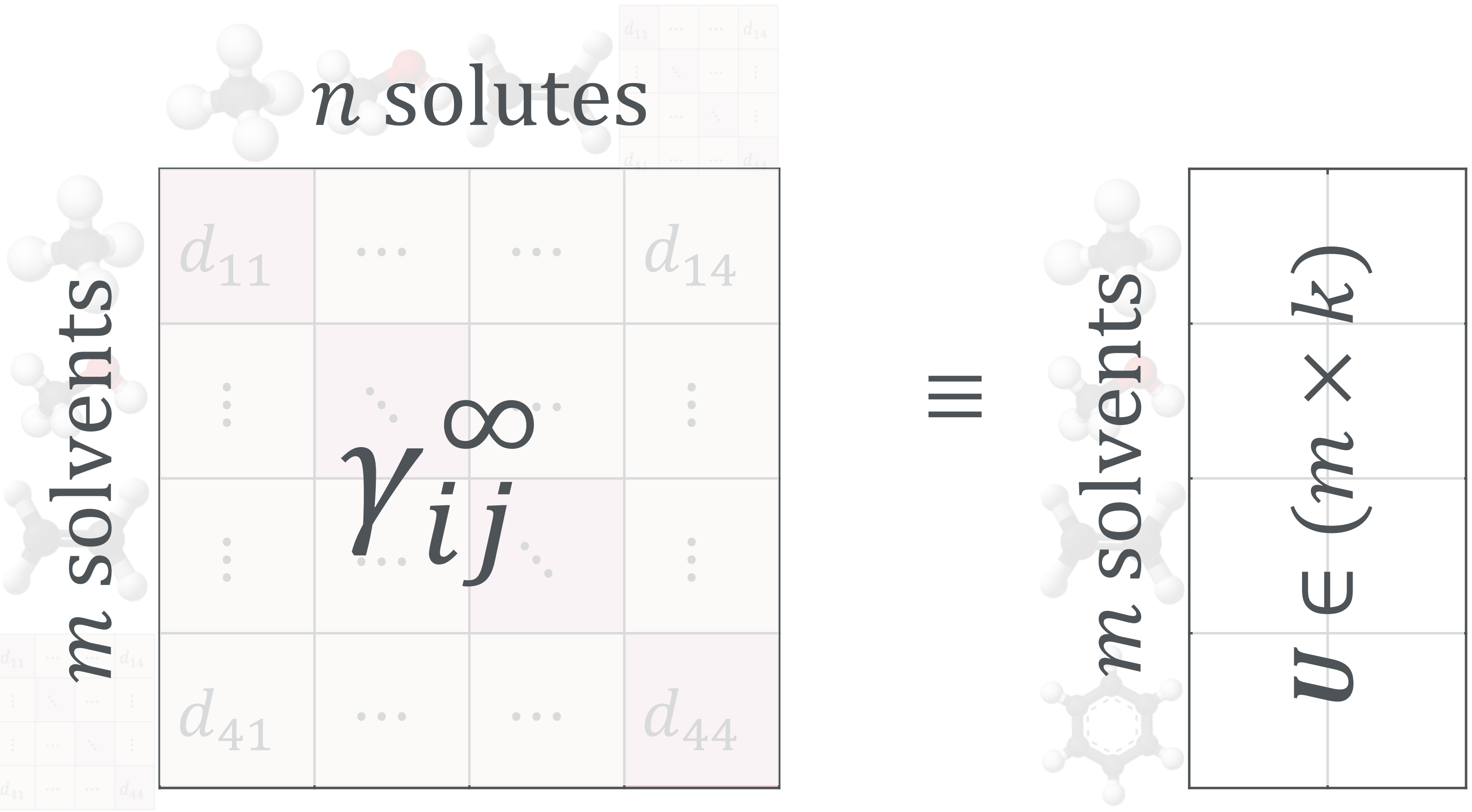
$U \in (250 \times k)$

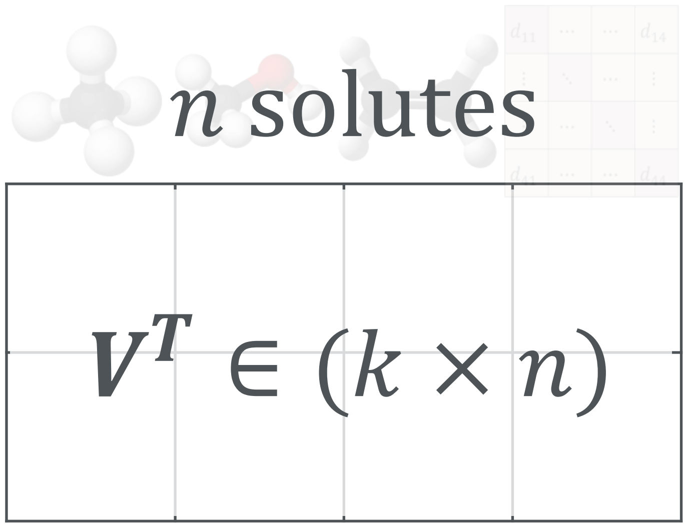
n solutes

$V^T \in (k \times 240)$

Success stories…

- Extended to other scalar valued mixture properties with similar success



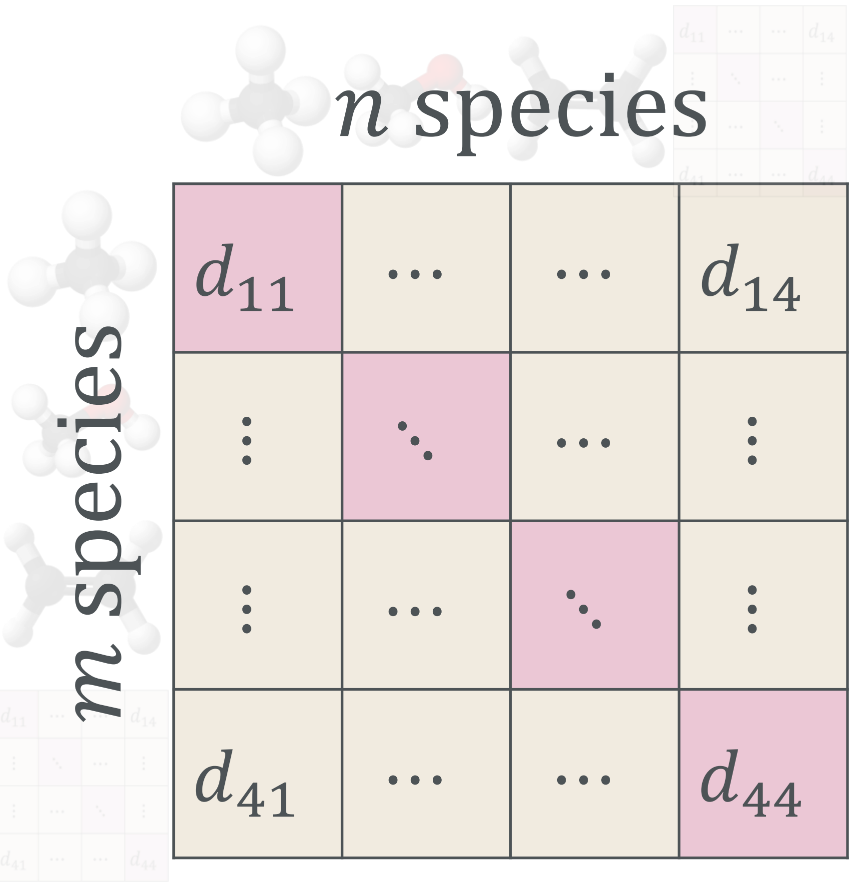


- Henry constants: H_{ij}
- Diffusion coefficient: D_{ij}
- UNIQUAC pair interactions: U_{ij}

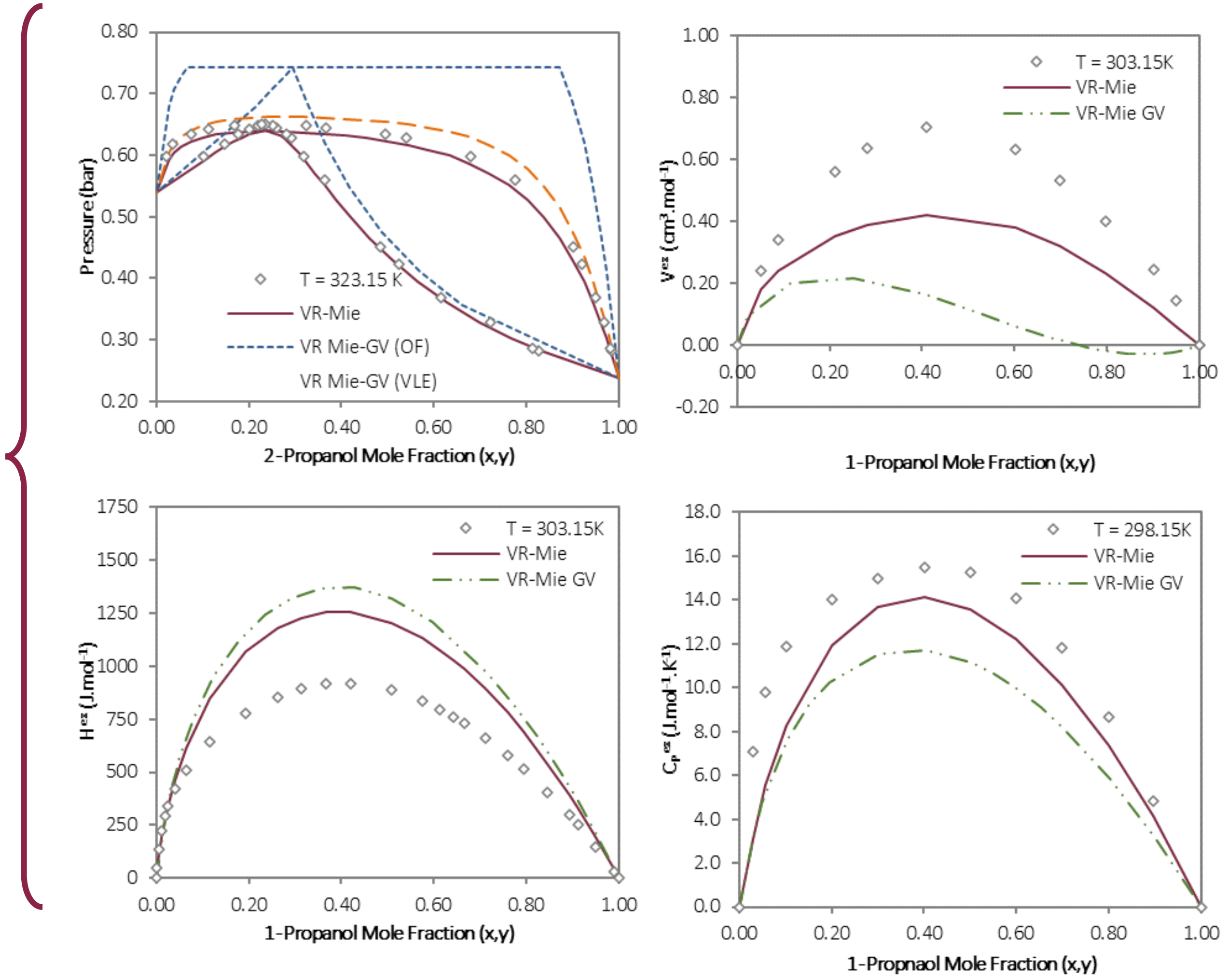
Hayer, N., et al. (2022). AIChE Journal 68(9)
Jirasek, F., et al. (2022). Chemical Science 13(17): 4854-4862
Großmann, O., et al. (2022). Digital Discovery 1(6): 886-897

Our interest…

- Higher dimensional data: composition (x_{ij}), temperature (T), pressure (P),…

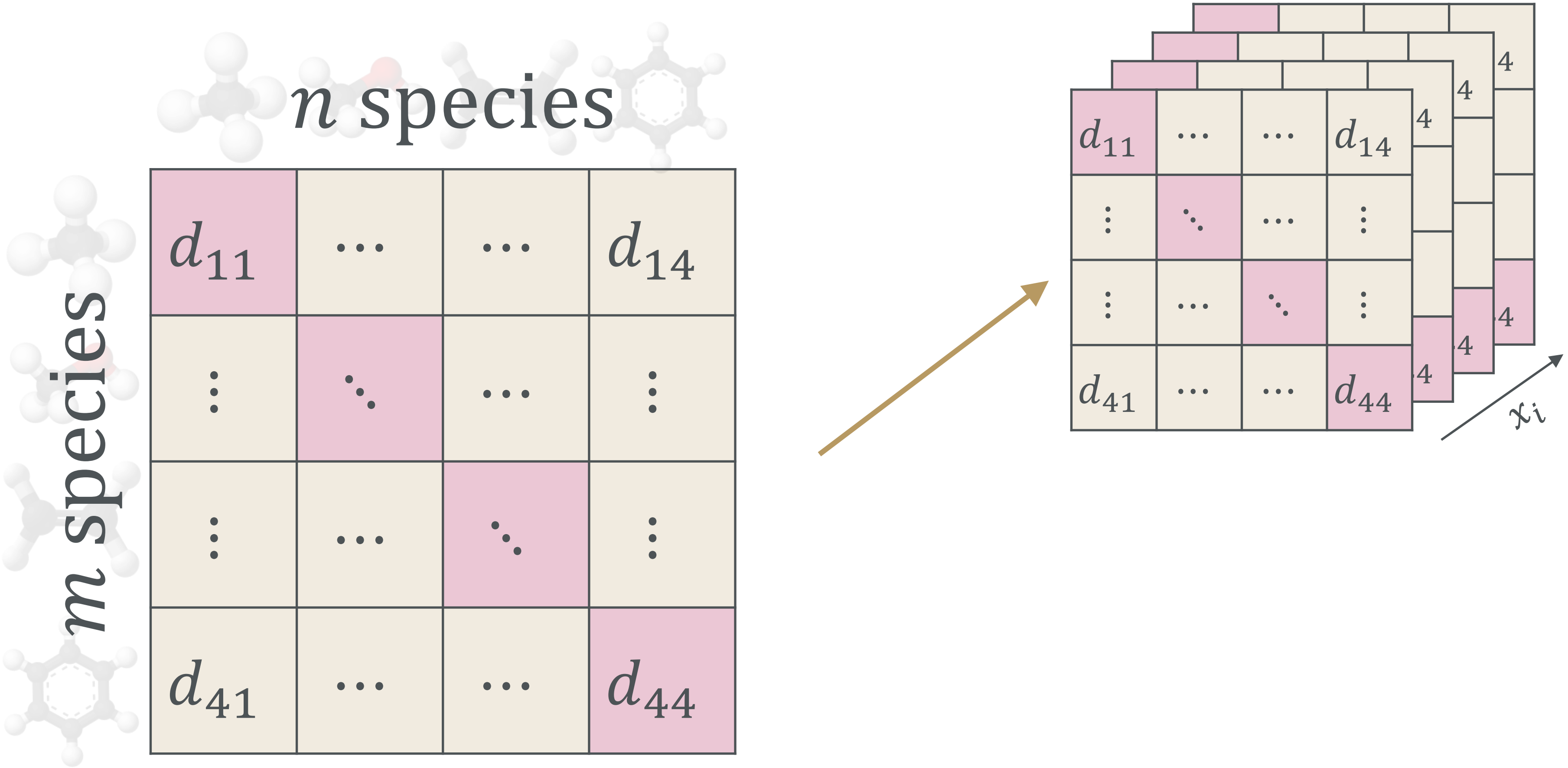


$\overset{?}{\longleftarrow}$



Our interest…

- **Higher dimensional** data: composition (x_{ij}), temperature (T), pressure (P),…

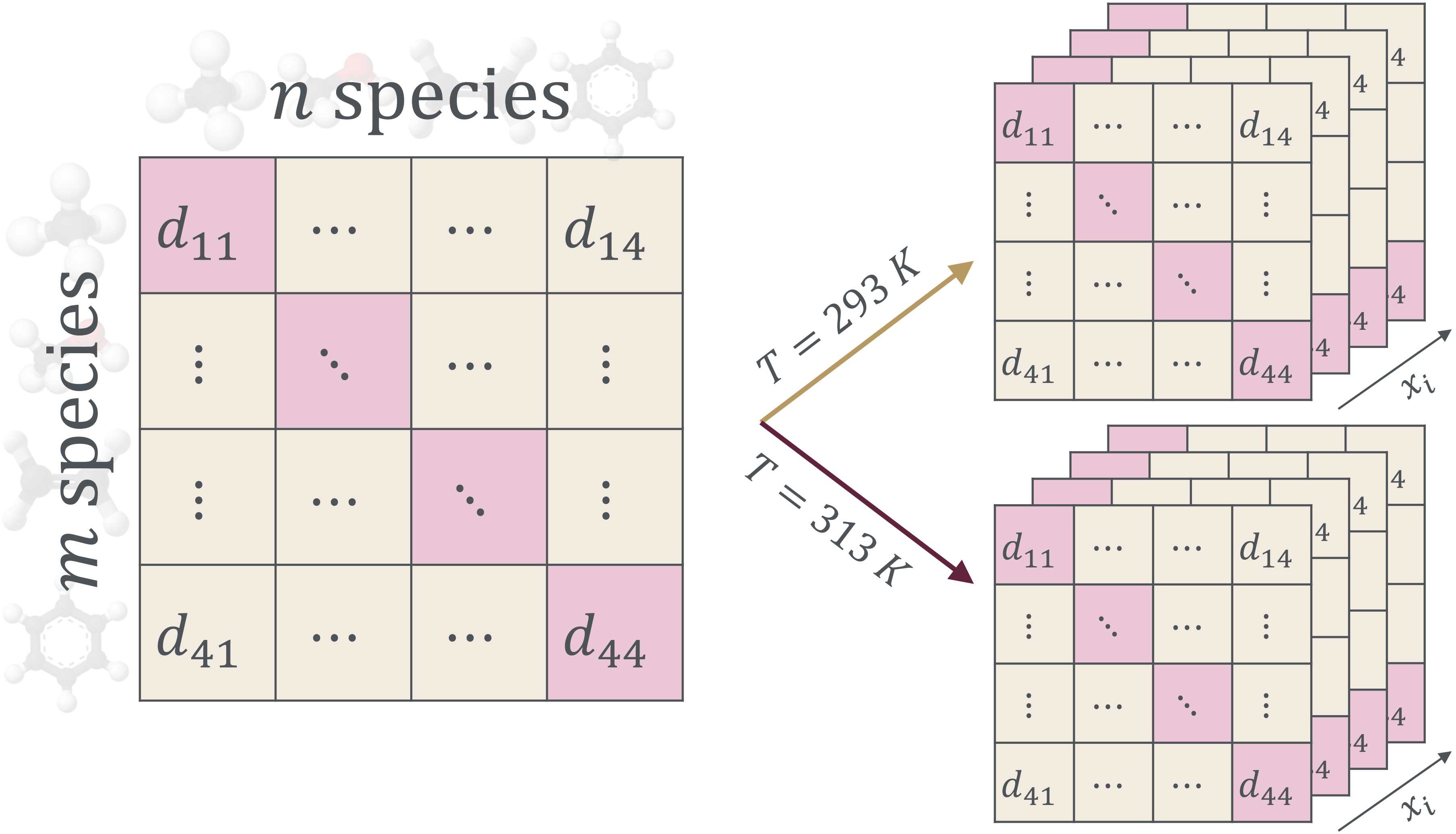


Parallelised Matrix Completion

- Independent "slices" of continuous, higher dimensions
- Same algorithm as MCM

Our interest…

- Higher dimensional data: composition (x_{ij}), temperature (T), pressure (P),…



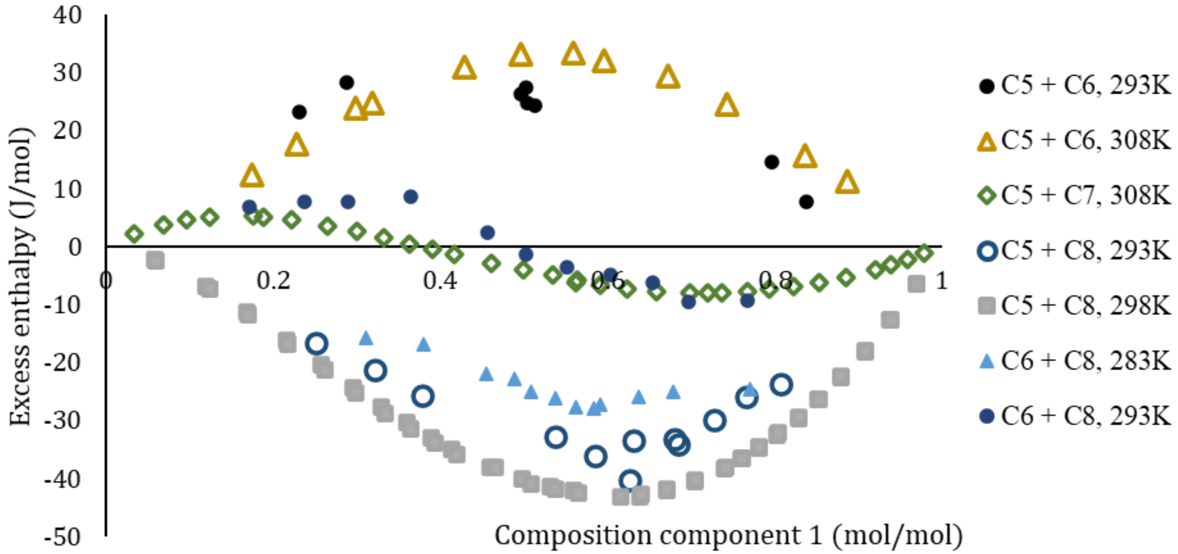
Parallelised Matrix Completion

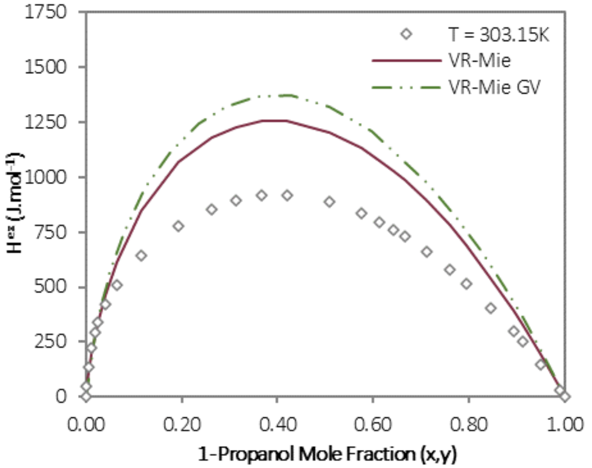
- Independent "slices" of continuous, higher dimensions
- Same algorithm as MCM

- Extra dimensions ≡ more "cubes"

The case for mixtures

- Liquid phase excess enthalpy (H^E):
  - monotonic, scalar valued, qualitatively varied
  - thermodynamic consistency testing, poorly predicted





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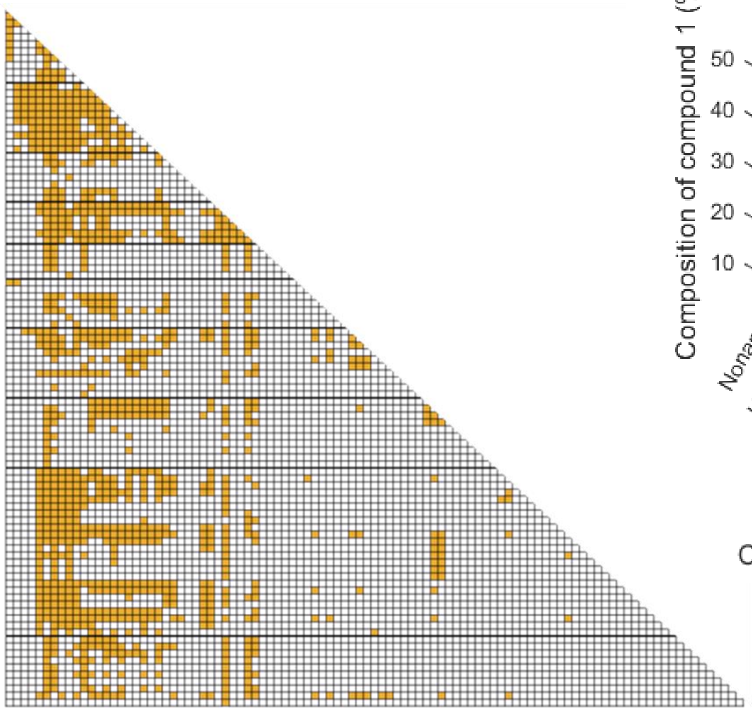
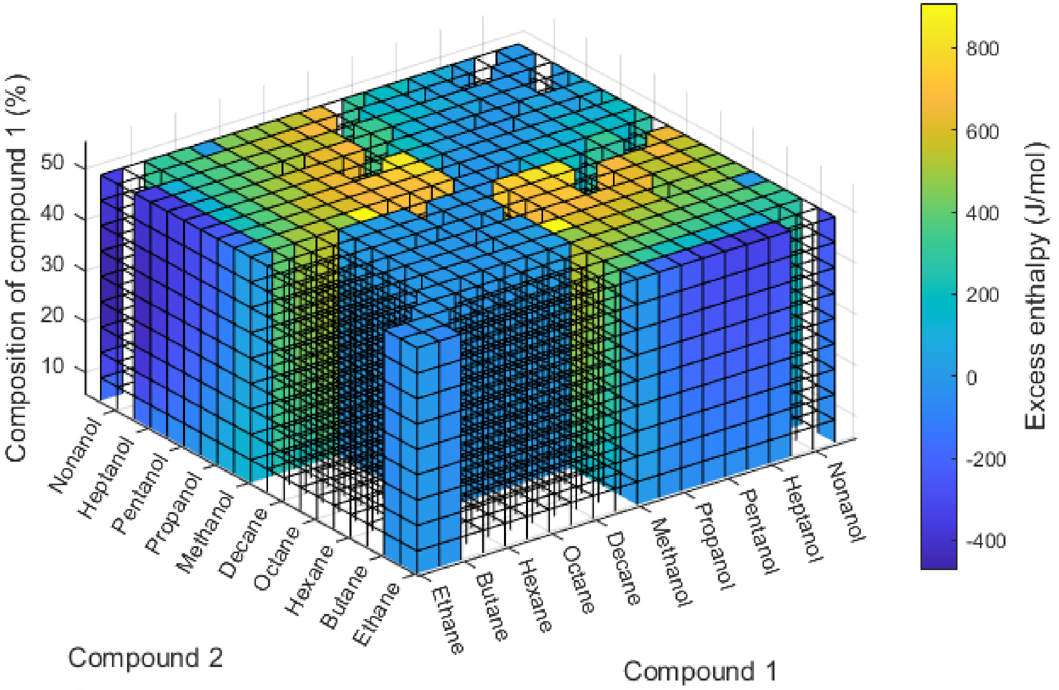
The case for mixtures

- Liquid phase excess enthalpy (H^E):
  - 97 components across 10 chemical families at 7 temperatures
  - 1012 mixtures from 4950 possible combinations → 11% - 20% observed





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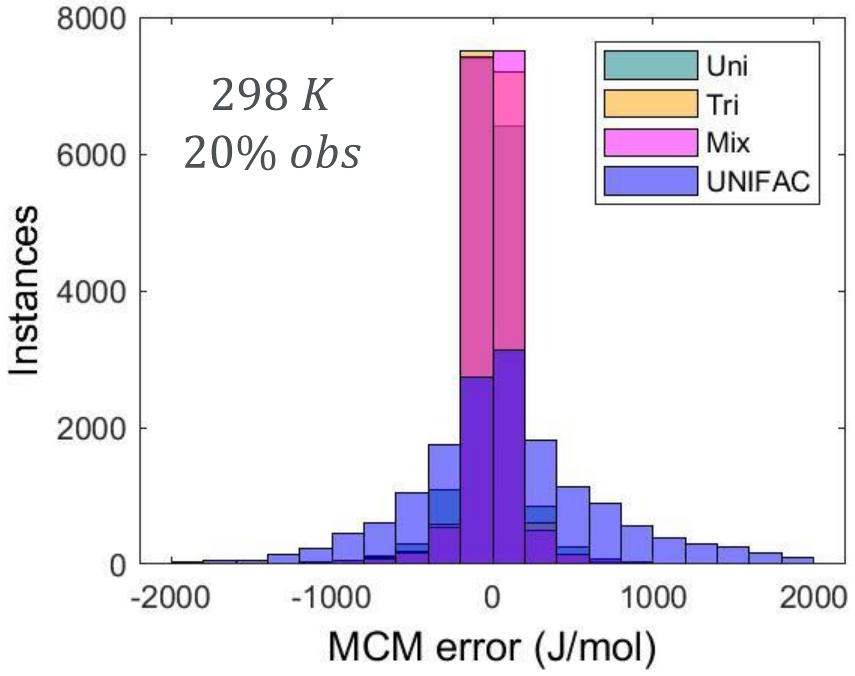
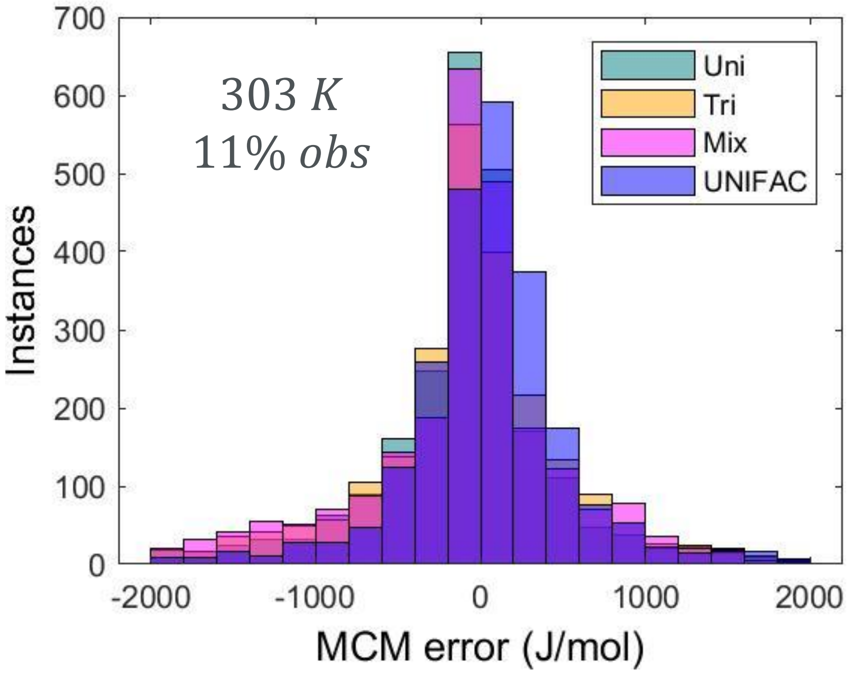
The case for mixtures

- More data ≡ better results
- More generalisable than UNIFAC Dortmund





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The case for mixtures

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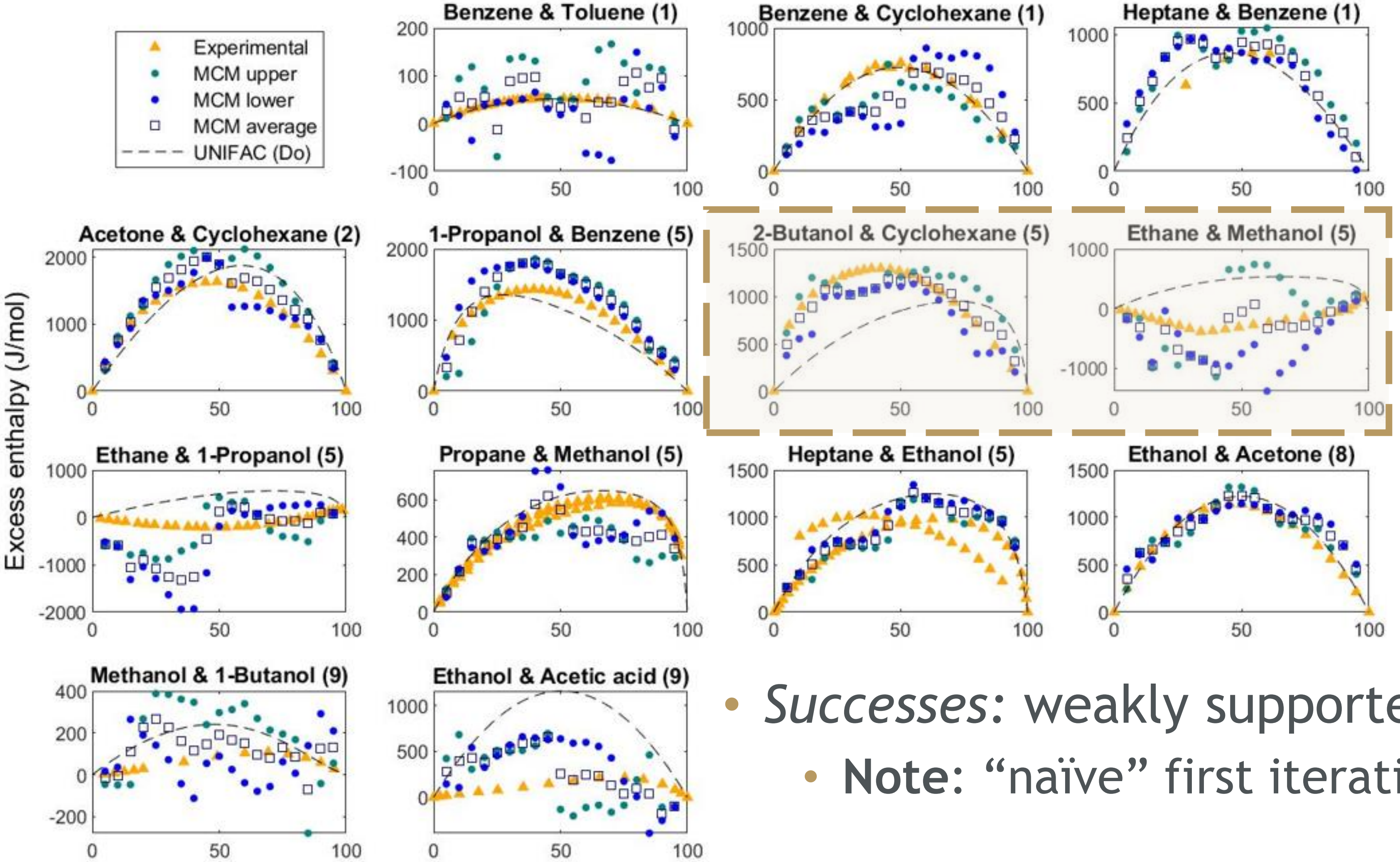

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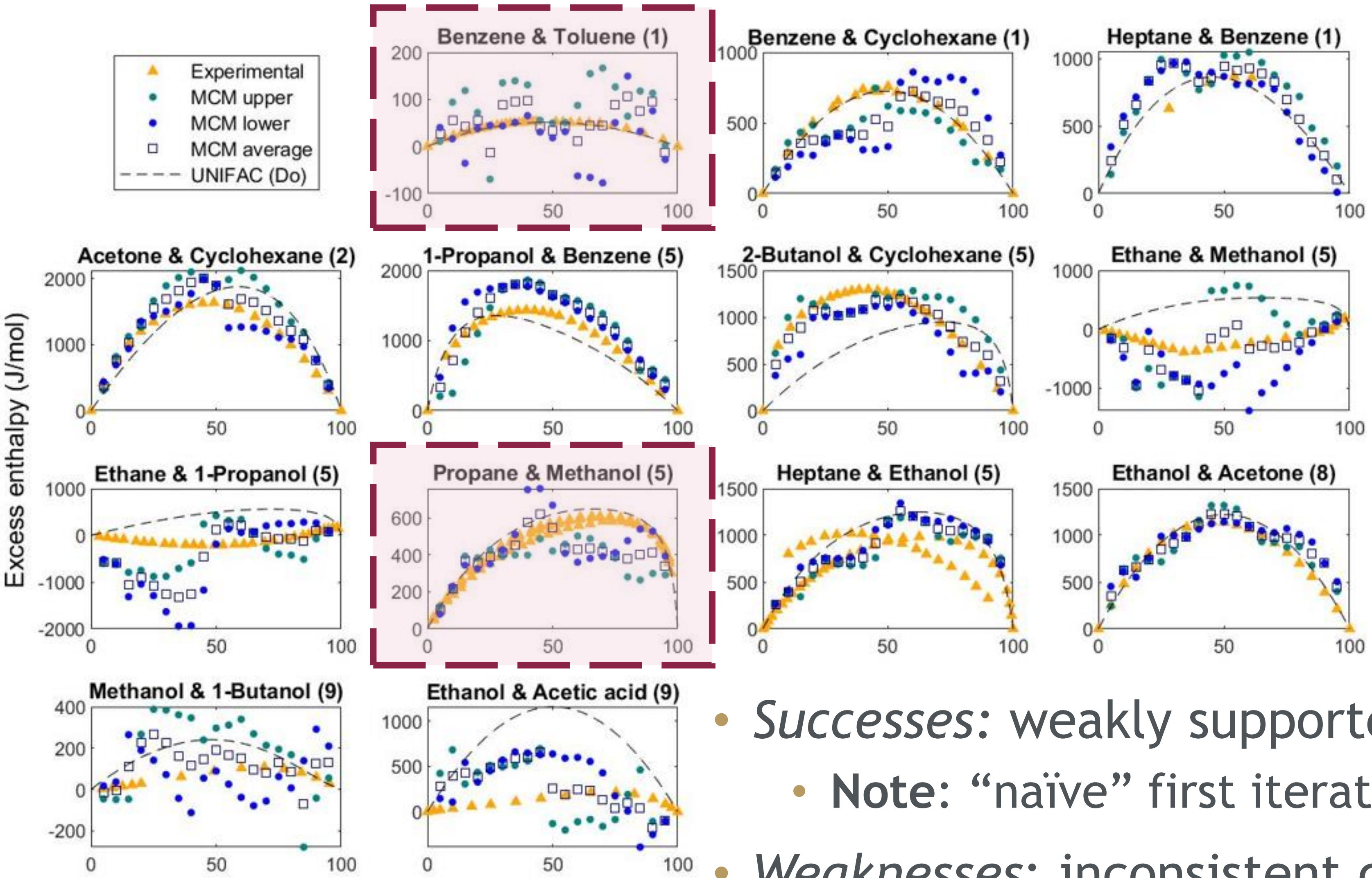
- *Successes*: weakly supported components; niche cases
  - **Note**: “naïve” first iteration

The case for mixtures



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- *Successes*: weakly supported components; niche cases
  - **Note**: “naïve” first iteration
- *Weaknesses*: inconsistent quality for “standard” systems; explicit trends in quality

Recommended for you…

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- Predictions not consistently quantitative
  - Won’t replace fundamental models

- Room for improvement
  - Hybrid models: incorporating predictive fundamental models
  - Alternatives: feature information, clustering
  - Quantifying uncertainty: probabilistic approach*

*Garren Hermanus

- Fundamentals first
  - Many hammers in machine learning toolbox, not all problems are nails…
  - Identify and understand problem → explore solutions
    - Chemical engineering, *then* machine learning…

Structured M.Eng (Chemical) with focus area: Data Analytics

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- Equip engineers with fundamentals of data science enabling application in the context of integrated industrial processes
- Collaboratively developed with industry
- Aimed at working engineers studying part-time
- Fully hybrid presentation
- 2024 intake ~ 20 students

Part-time students	Term 1	Term 2	Term 3	Term 4	*Full-time students*
Year 1	Data Science	Applied Machine Learning	Plantwide Dynamics andControl		Year 1
Year 2	Numerical Methods	Optimisation		Data Analysis for Dynamic Processes	
Year 3	Advanced Topics in Eng. Management Integrated Process Data Analysis	Research project			Year 2

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Thank you
Enkosi
Dankie

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