Artificial intelligence-driven design of fuel mixtures

Nursulu Kuzhagaliyeva[1], Samuel Horvath[2], Andre Nicolle[3], S. Mani Sarathy[1]
[1]Clean Combustion Research Center, KAUST, [2] Visual Computing Center, KAUST, [3] Aramco Fuel Research center, France

KAUST Research Conference:
AI for Energy
6-8 March 2023

Why fuel design is needed?

- Transport sector is responsible for nearly 25% of total CO_2 emissions
- By 2040, 75% of light-duty vehicles globally will still have ICE engines

Climate change mitigation urges the formulation of **low carbon transportation fuels**.

Promising new blendstocks

High efficiency fuels

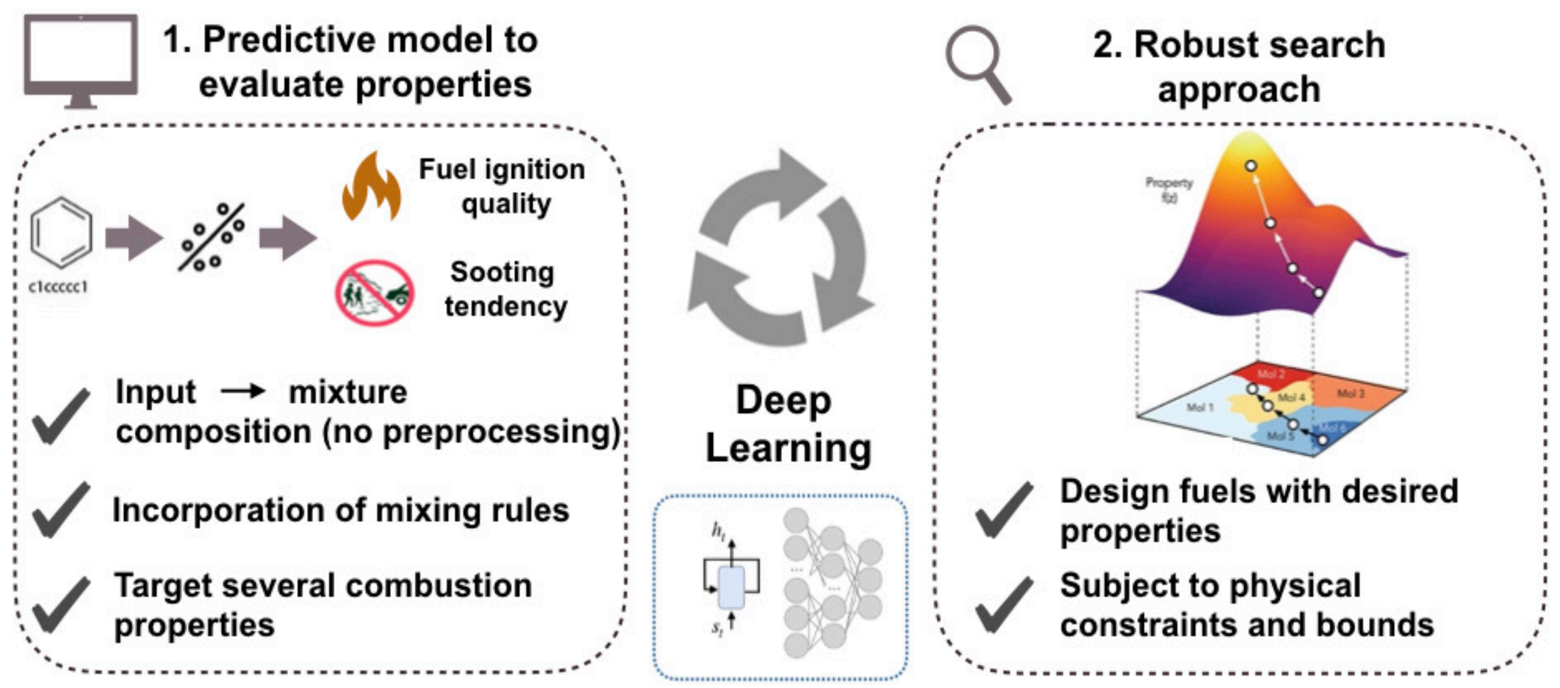
Reduced emissions

Conventional tools
- Cyclic, timely, and costly
- Multistep fuel design process
- Requires trial and error

AI tools
- Mostly for single components
- Needs pre-processing (blends)
- Not suitable for inverse design

Inverse fuel design framework

Can be implemented as a constrained optimization task



Prediction of mixtures properties remains **one of the key bottlenecks for the inverse fuel design**

Methodology

1. Data curation

- **Pure species → 19 molecular classes**
- **Oxygenates → 20 and 50% of ON and YSI databases**
- **76 complex mixtures**

Table 1. Curated database for RON, MON and YSI

		RON[1]	MON[2]	YSI[3]
Pure species	OC[4]	74	67	221
	NON-OC	290	266	231
	total	364	333	452
Blends	≤10 comp.	372	293	35
	>10 comp.	76	64	5
	total	448	357	40
Total		812	690	492

[1]Reseach Octane Number , [2]Motor Octane Number , [3]Yield Sooting Index, [4]Oxygenated compounds

2. Joint-properties predictive network

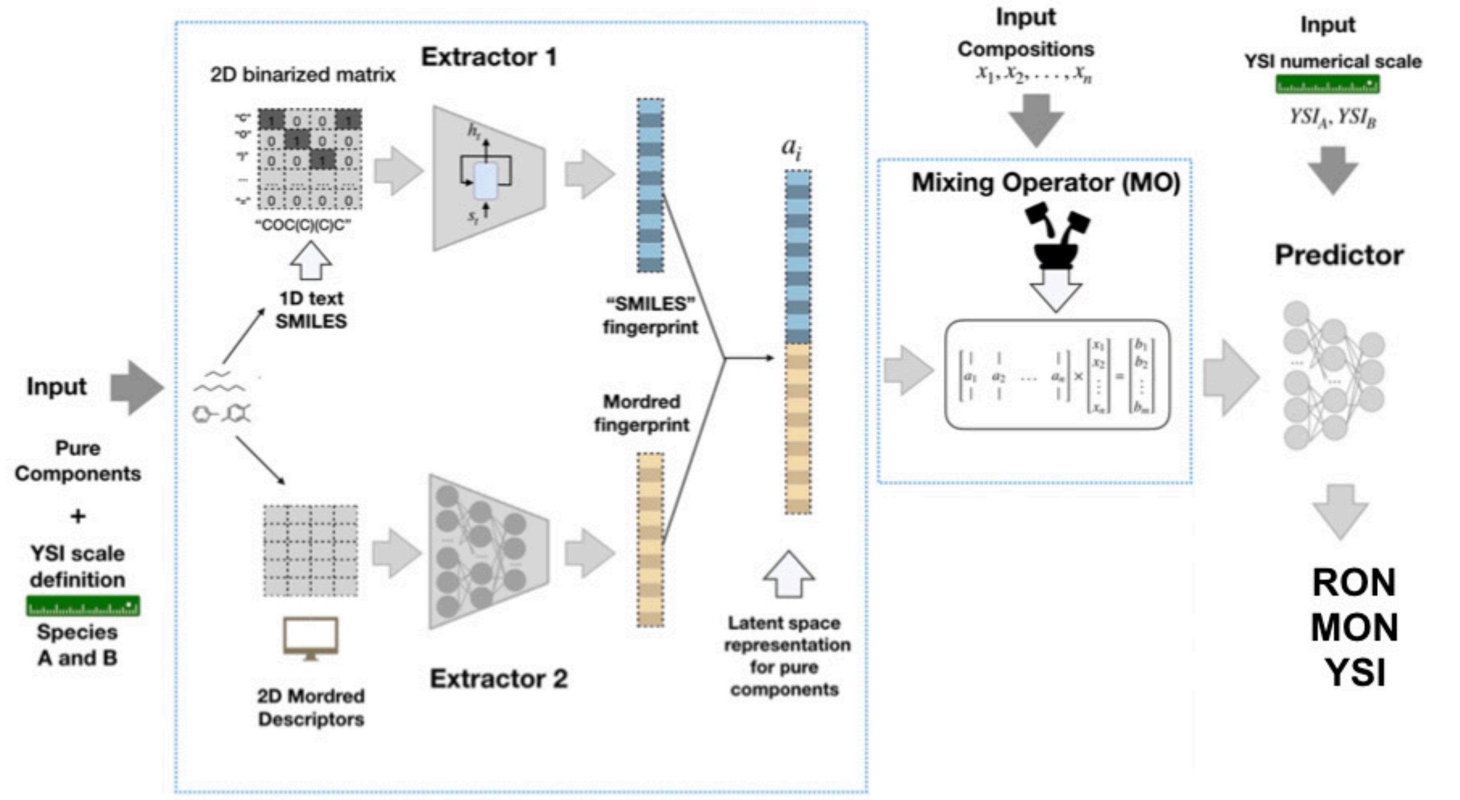
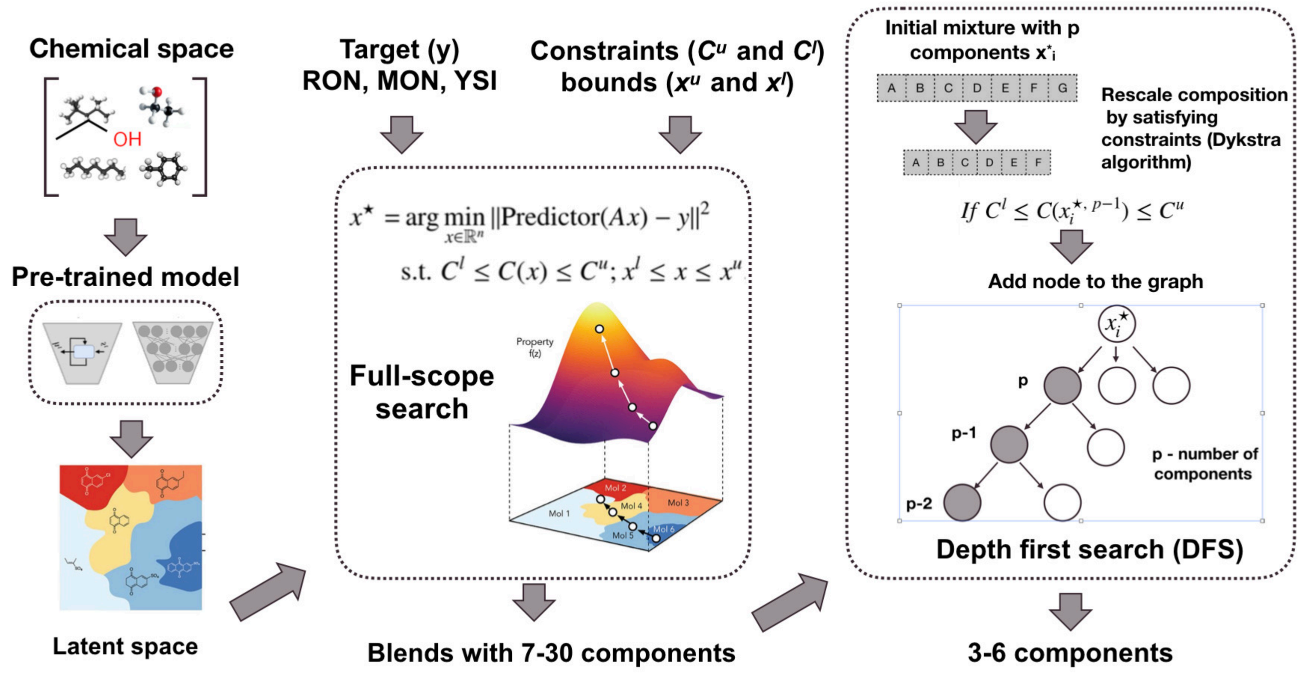


Fig 1. Skeletal network architecture for joint-properties predictive model for pure components and mixtures.

3. Two search approaches to formulate mixtures with desired properties and subject to physical constraints



Results

1. Performance on test set

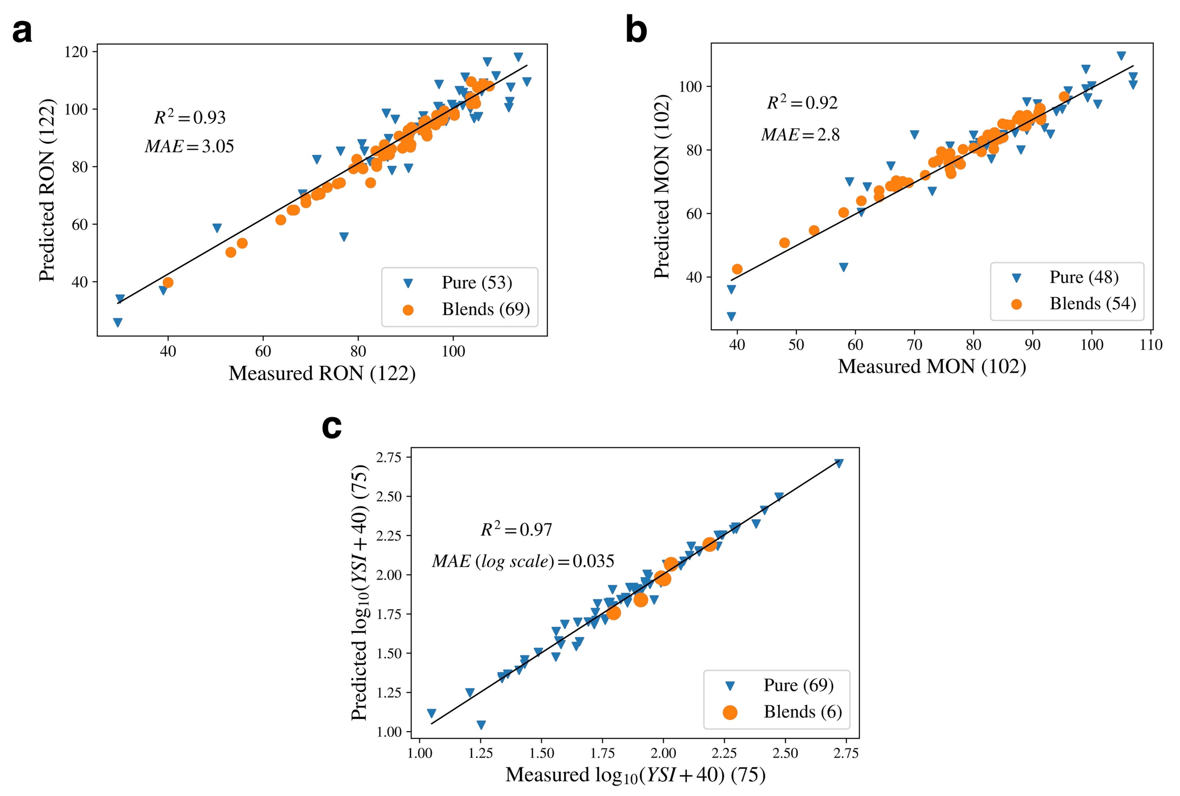


Fig 2. Parity plots for **a** RON, **b** MON and **c** YSI in log scale.

Table 3. Supplementary properties of new potential components from short-listed mixtures.

Compound	FKMC	EPIB7	WS (gL^{-1})	AHL (d)	MP (°C)
Tetramethoxy methane	yes	-0.845	110	3.2	-5
Isopentyl acetate	Yes (if<5%)	0.655	2.0	1.8	-78
Ethylidene cyclopentane	yes	0.203	0.1	0.12	-129

*Notation: FKMC = FKM compatibility, EPIB7 = EPI Biowin 7, WS = Water solubility, AHL = Atmospheric half-life, MP = Melting point.

2. Analysis of obtained blends (RON=95, MON=85, YSI=60, gasoline specifications)

Table 2. Short list of mixtures exhibiting acceptable RVP(50-100 kPa)

Mixture	RVP (kPa)	LHV MJ/kg	Viscosity mPa*s	Density °C
17-1	78.7	38.2	1.11	1.04
22-13	50.3	40.3	1.36	0.751
18-17	67.4	39.7	0.77	0.791
26-20	52.5	37.8	1.2	0.785
6-1	61.0	42.4	0.65	0.732

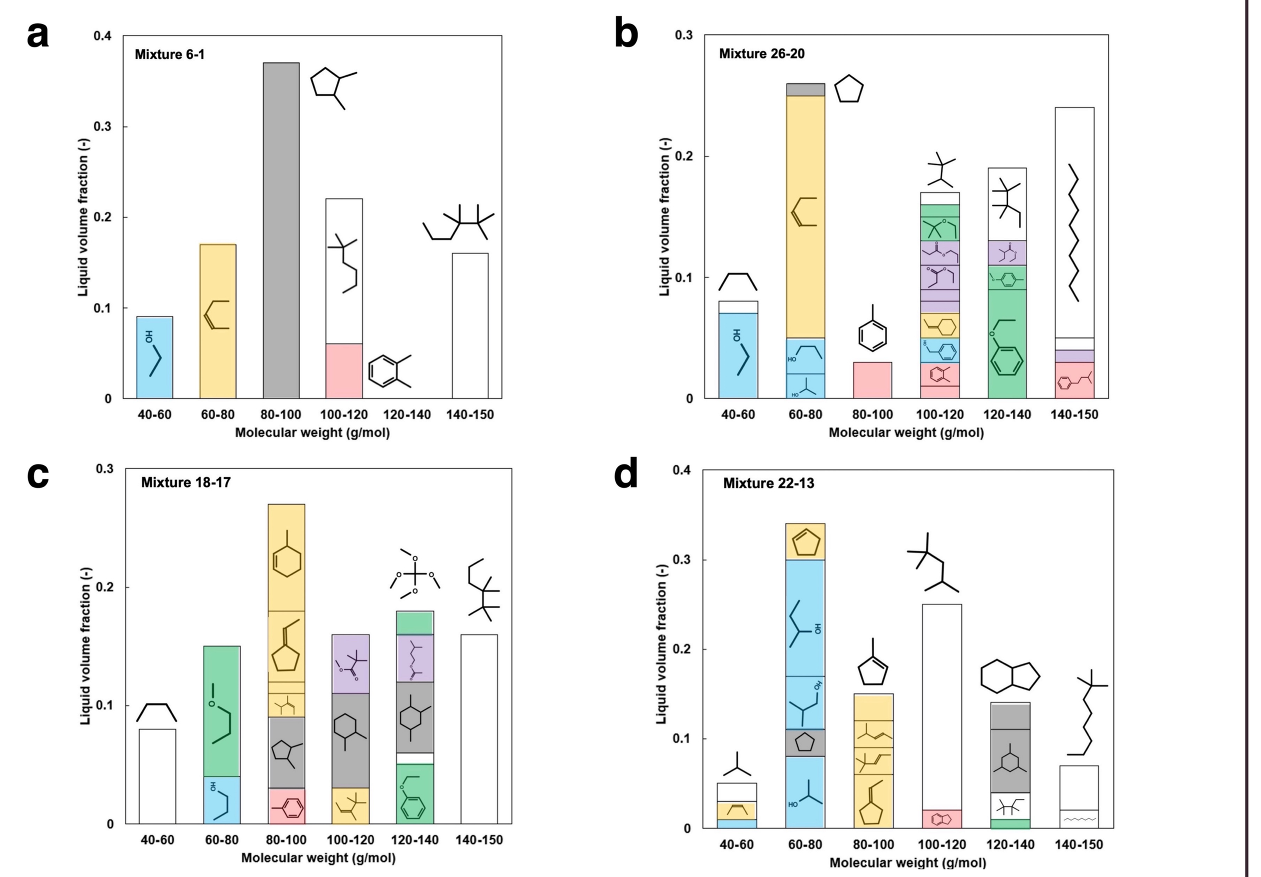


Fig 3. Molecular weight distributions of 4 mixture candidates with predicted RON/MON/YSI

Summary

- Comprehensive database was curated for pure components and mixtures
- Joint-properties predictive model for pure components and mixtures
- 2 search algorithms to formulate fuels with desired properties

Work in progress

- Extend property database (volatility (Reid Vapor Pressure), density, LHV)
- Implement state-of-the art architectures (GNN)
- Pollutants screening using low dimensional models