Technical University of Denmark

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DESIGN OF FEASIBLE BLENDS OF GASOLINE AND BIOFUELS USING A SYSTEMATIC COMPUTER AIDED TECHNIQUE

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BY:
NOR ALAFIZA YUNUS

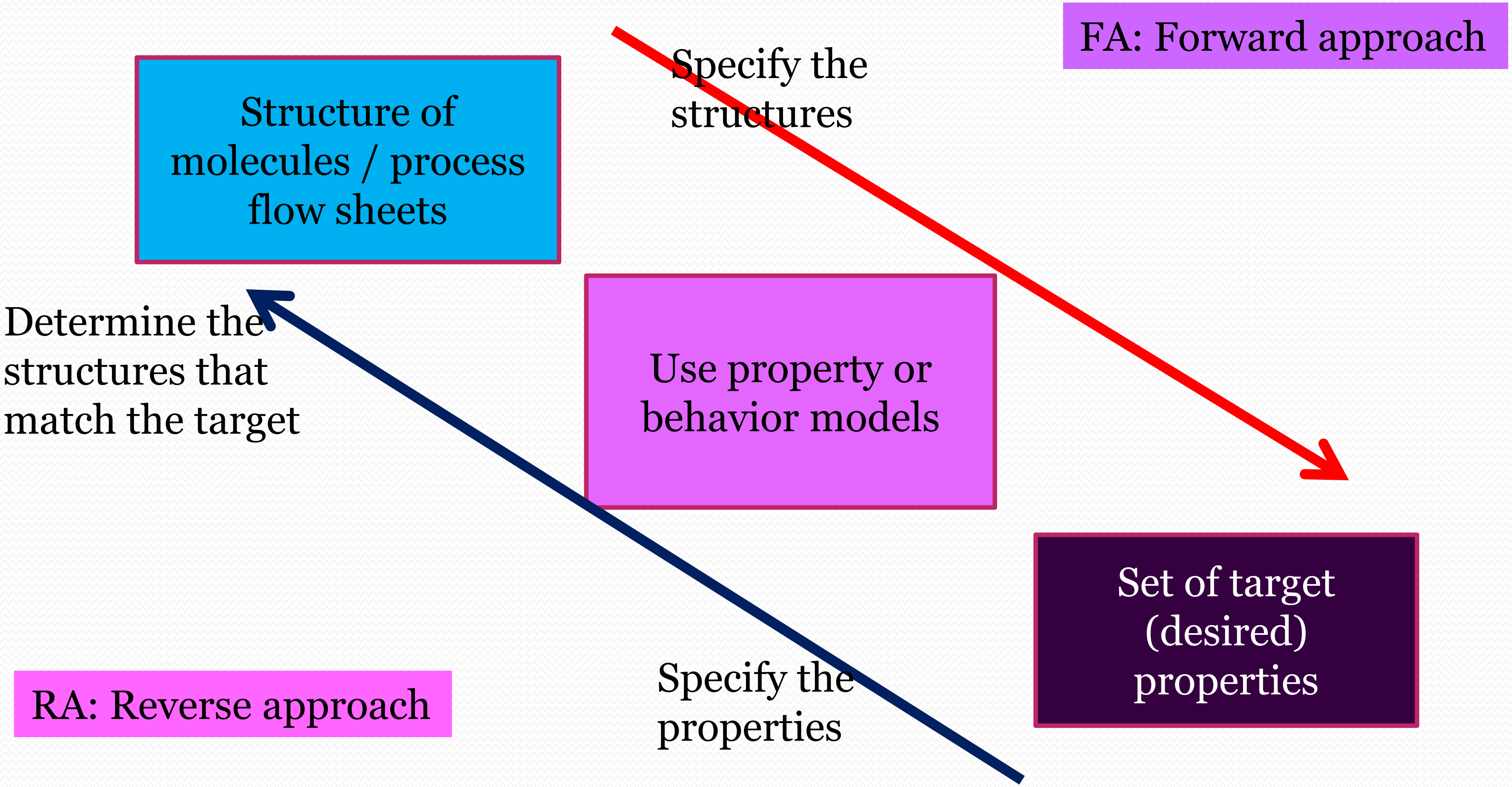
Outline

- Introduction
- Motivation
- Objective
- Methodology
- Results
- Future work

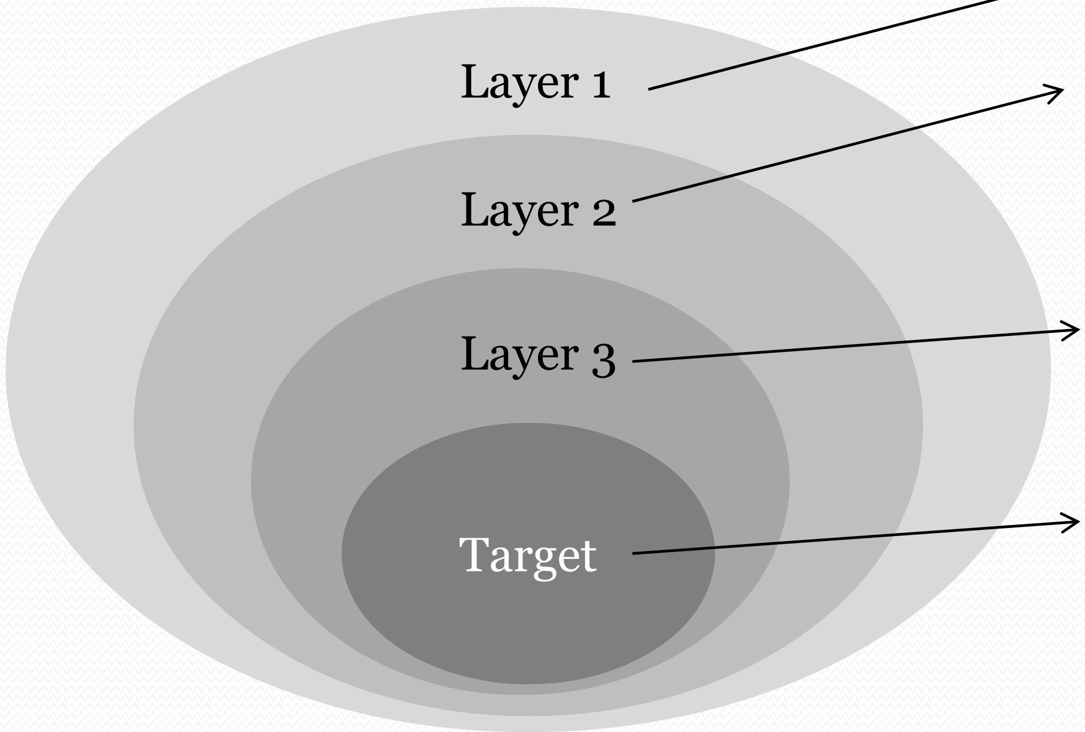
CAPEC

Introduction

Chemical Product Design

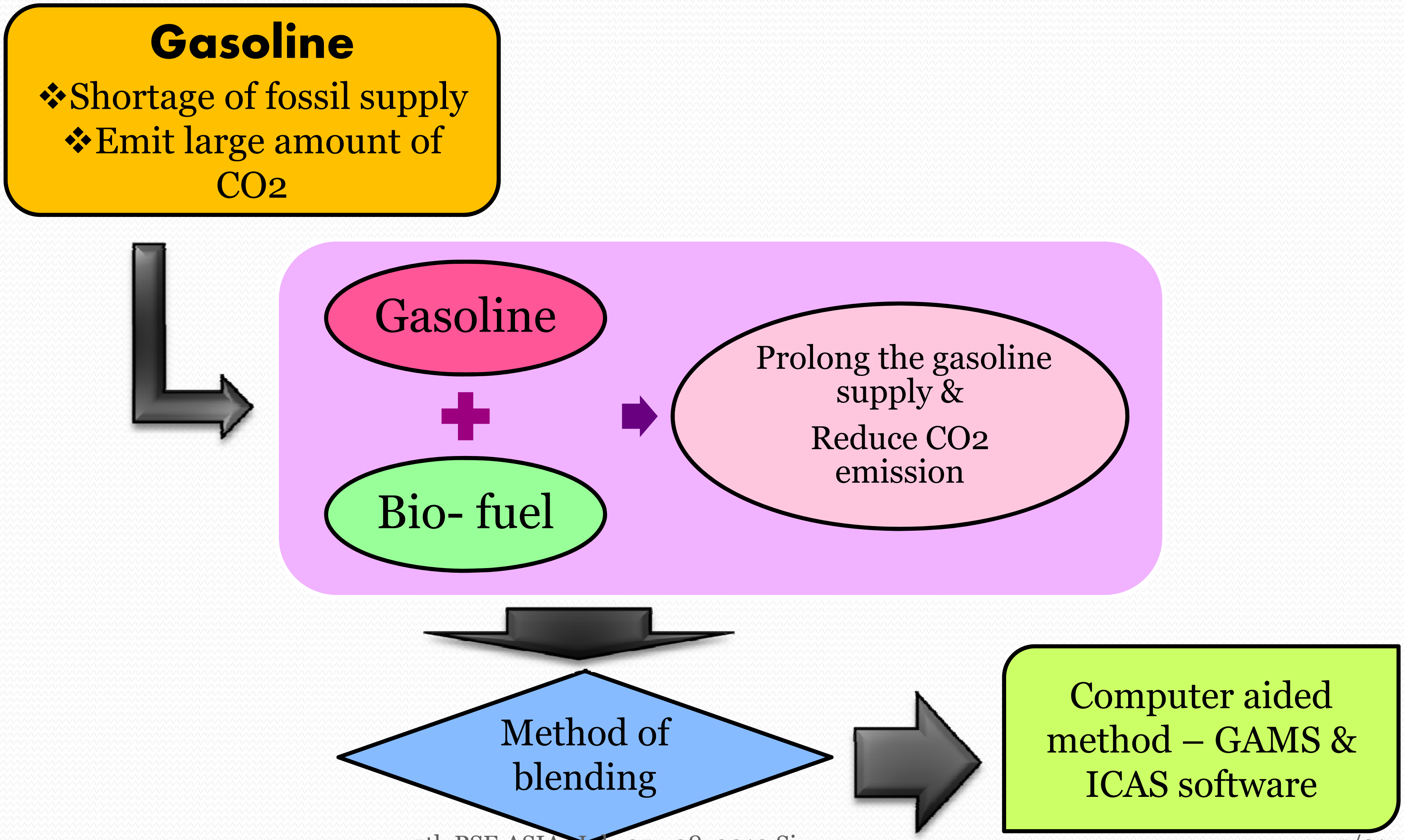


Introduction



- Layer 1: Start searching at bigger space
- Layer 2: Reduce searching space when a constraint was introduce – eliminate unwanted candidates
- Layer 3: Further reduce searching space when more constraints were introduce
- Target area: Finally, the right candidate was able to find at a small target area

Motivation


Gasoline
❖Shortage of fossil supply
❖Emit large amount of CO2
Gasoline
Bio- fuel
Prolong the gasoline supply &
Reduce CO2 emission
Method of blending
Computer aided method – GAMS & ICAS software

Objective

To find a set of feasible blend of gasoline and bio-fuel which are could reduce fossil fuel consumption using a systematic computer aided approach

Methodology

Step 1 — Identify target properties and target values

Step 2 — Identify properties model

Step 3 — Identify the possible blend mixture

Step 4 — Generate the possible blend candidates

Step 5 — Validate the model

Methodology

step	Task	Method & tools	Output
1	Identify the important target property	Literature (journals) Blending guideline	List of target properties
	Set the target value for each target property	Literature (journals), Blending regulation Existing product	List of constraints
2	Identify pure and mixture property model	Literature, calculated directly from chemical structure	Pure property models Mixture property models
3	Identify the feasible mixture	ICAS	List of feasible blend compositions
4	Generate the possible mixture candidates	GAMS	List of several possible mixture candidates
5	Model validation	Experiment	Experimental data

ICAS: Integrated Computer Aided System

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Methodology

- Step 1 — Identify target properties and target values
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Property	Target value
Heating Value	> 35 MJ/kg
Octane number	> 90
Density	700 – 790 kg/m^3
Kinematic viscosity	< 2.41 mm^2/s

Methodology

- Step 1: Identify target properties and target values
- **Step 2: Identify properties model**
- Step 3: Identify the possible blend mixture
- Step 4: Generate the possible blend candidates
- Step 5: Validate the model

Property	Model
Heating Value	$HV_{mix} = \sum x_i HV_i$
Octane number	$ON = \sum x_i ON_i$
Density	$\rho_{mix} = \sum x_i \rho_i$
Kinematic viscosity	$\nu_{mix} = \frac{1}{\rho_{mix}} \exp\left(\sum \upsilon_i \ln \eta_i\right)$

Methodology

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PT-flash (multiphase) calculation

Thermodynamic model

Soave-Redlich-Kwong

ICAS 11

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Methodology

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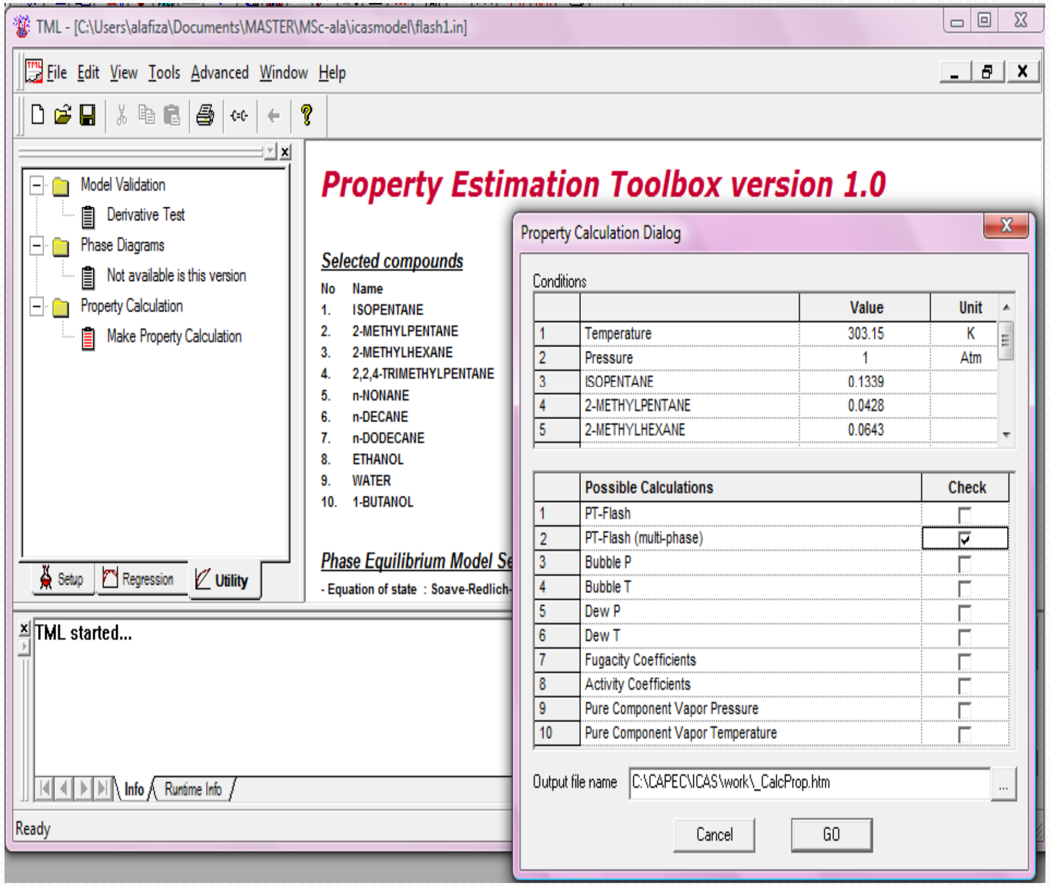
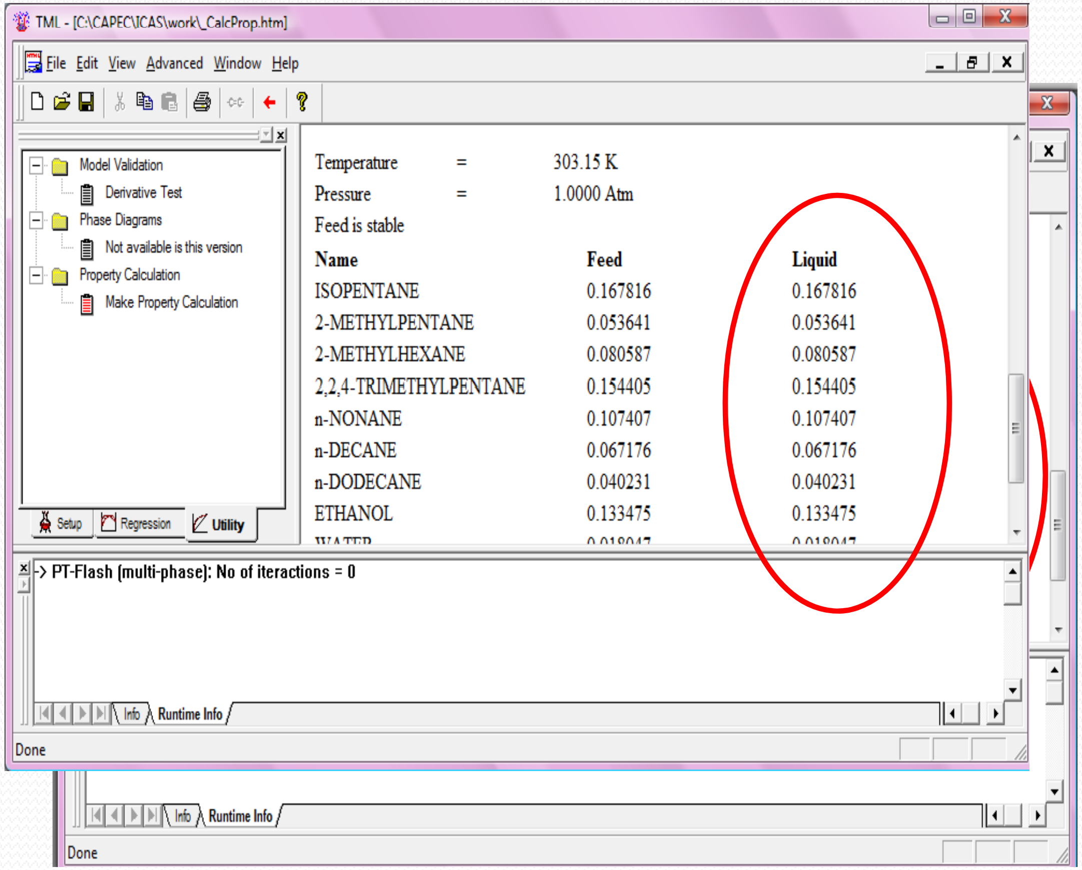


Methodology

- **Step 1** Identify target properties and target values
- **Step 2** Identify properties model
- **Step 3** Identify the possible blend mixture
- **Step 4** Generate the possible blend candidates
- **Step 5** Validate the model



Methodology

Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model

Using GAMS (General Algebraic Modeling System)

Property constraint:

$HV = \sum x_i HV_i$

$ON = \sum x_i ON_i$

$\rho_{mix} = \sum x_i \rho_i$

$$\nu_{mix} = \frac{1}{\rho_{mix}} \exp\left(\sum \upsilon_i \ln \eta_i\right)$$

Volume constraint

$V_{gasoline} \geq 0.5$

$V_{ethanol} \leq 0.05$

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Methodology

- Step 1 Identify target properties and target values
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Target Properties	ρ (kg/m^3)	ν (mm^2/s)	HHV (KJ/kg)	Wt % O_2	ON
Gasoline	686.85	0.71	48028	0.00	95
Ethanol	769.84	1.84	29136	34.00	110
Butanol	805.89	3.15	36212	21.60	102.74
MTHF	808.20	0.36	36059	18.57	112.2

Methodology

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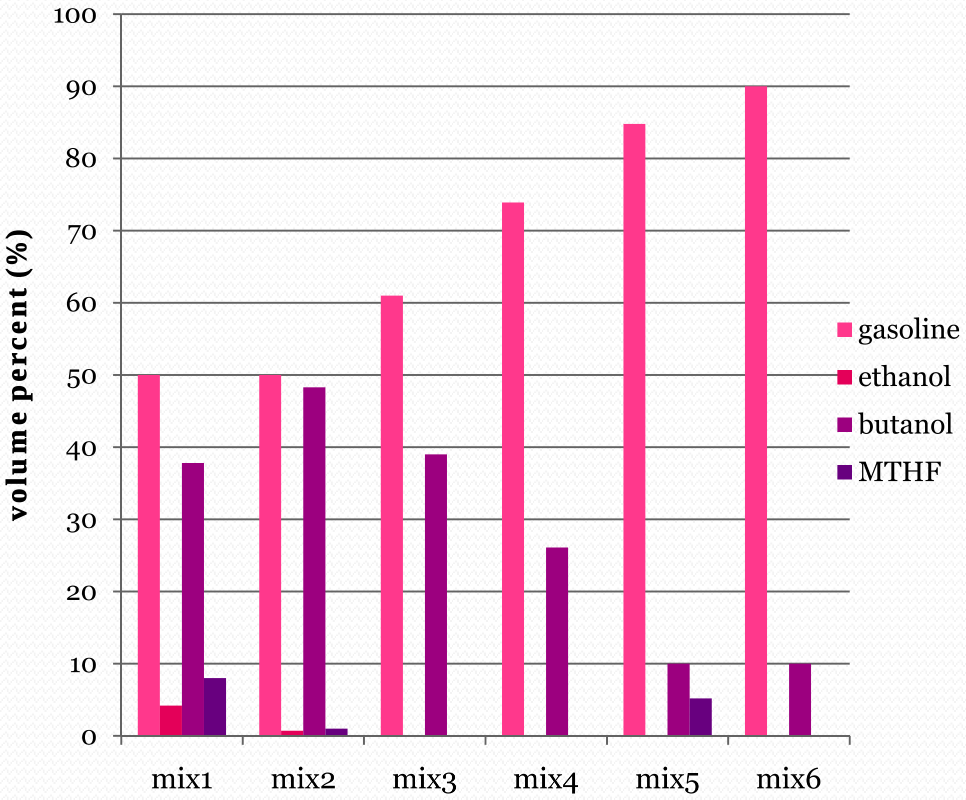
Future work

Results

Composition	Mix 1	Mix2	Mix3	Mix4	Mix5	Mix6
Gasoline	0.500	0.500	0.610	0.739	0.848	0.90
Ethanol	0.042	0.007				
Butanol	0.378	0.483	0.390	0.261	0.100	0.10
MTHF	0.08	0.010			0.052	
Property						
HV	41.167	41.473	42.779	44.414	45.945	46.746
Density	749.156	749.130	736.186	720.522	707.696	700.000
Viscosity	0.00152	0.00174	0.0016	0.00138	0.00106	0.00109
ON	100	99	98	97	96	95

Results



- All candidates consist of butanol
- Butanol is most favorable component due to attractive characteristics
- It has higher energy content which is close to gasoline energy content, less prone to water contamination and less corrosive

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Conclusion

- A systematic computer aided technique is a resources efficient technique which is suitable to find a set of target candidates
- Property model availability is one of the challenges in chemical product design

Future work

- Including emission factor to produce a green fuel
- Model validation through a series of experimental work

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THANK YOU
Q&A session