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

Nor Alafiza Yunus, Zainuddin Abd. Manan,
Haslenda Hashim and Rafiqul Gani

BY:

NOR ALAFIZA YUNUS

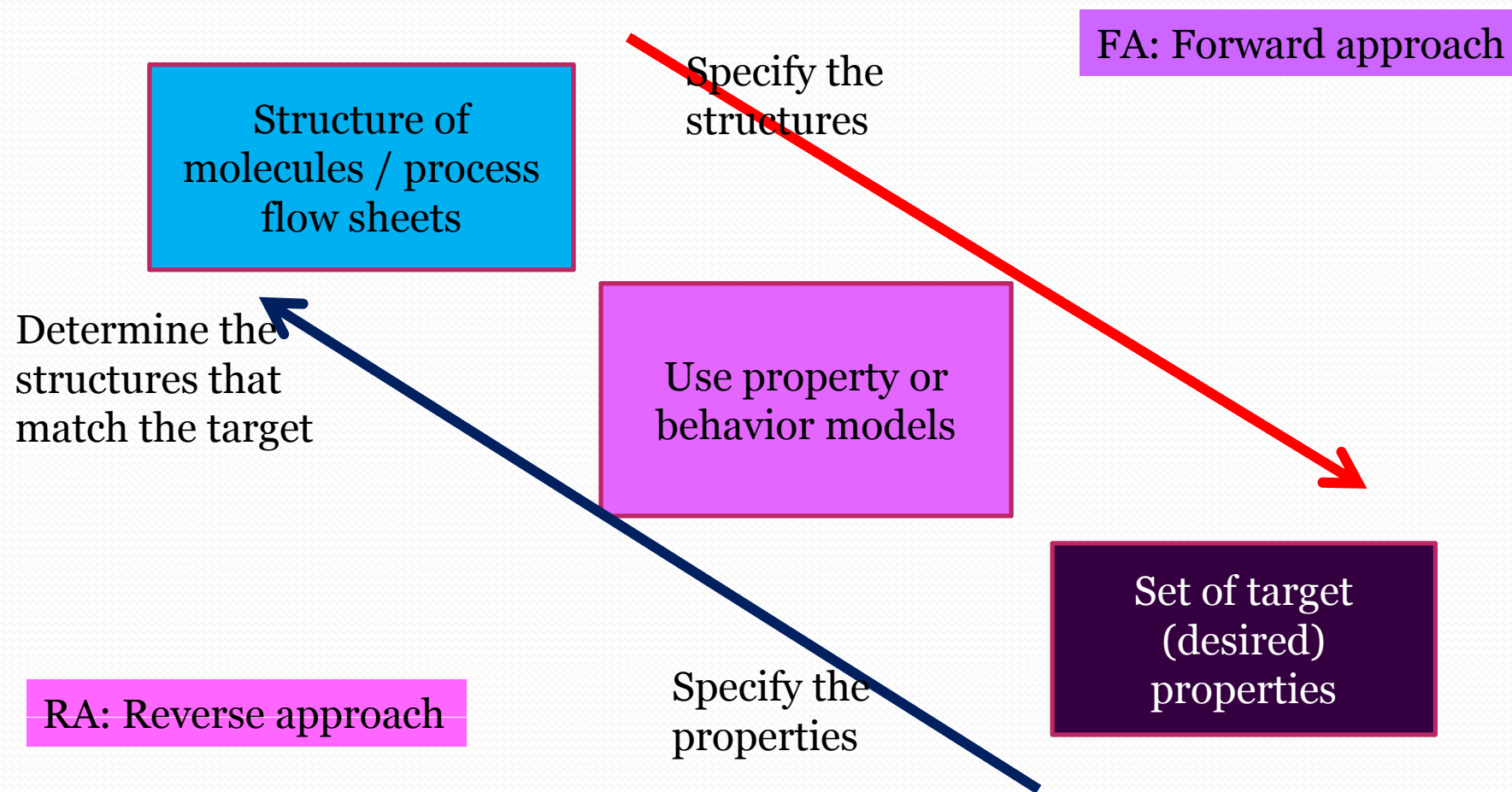
5th PSE ASIA, July 25 - 28, 2010 Singapore

Outline

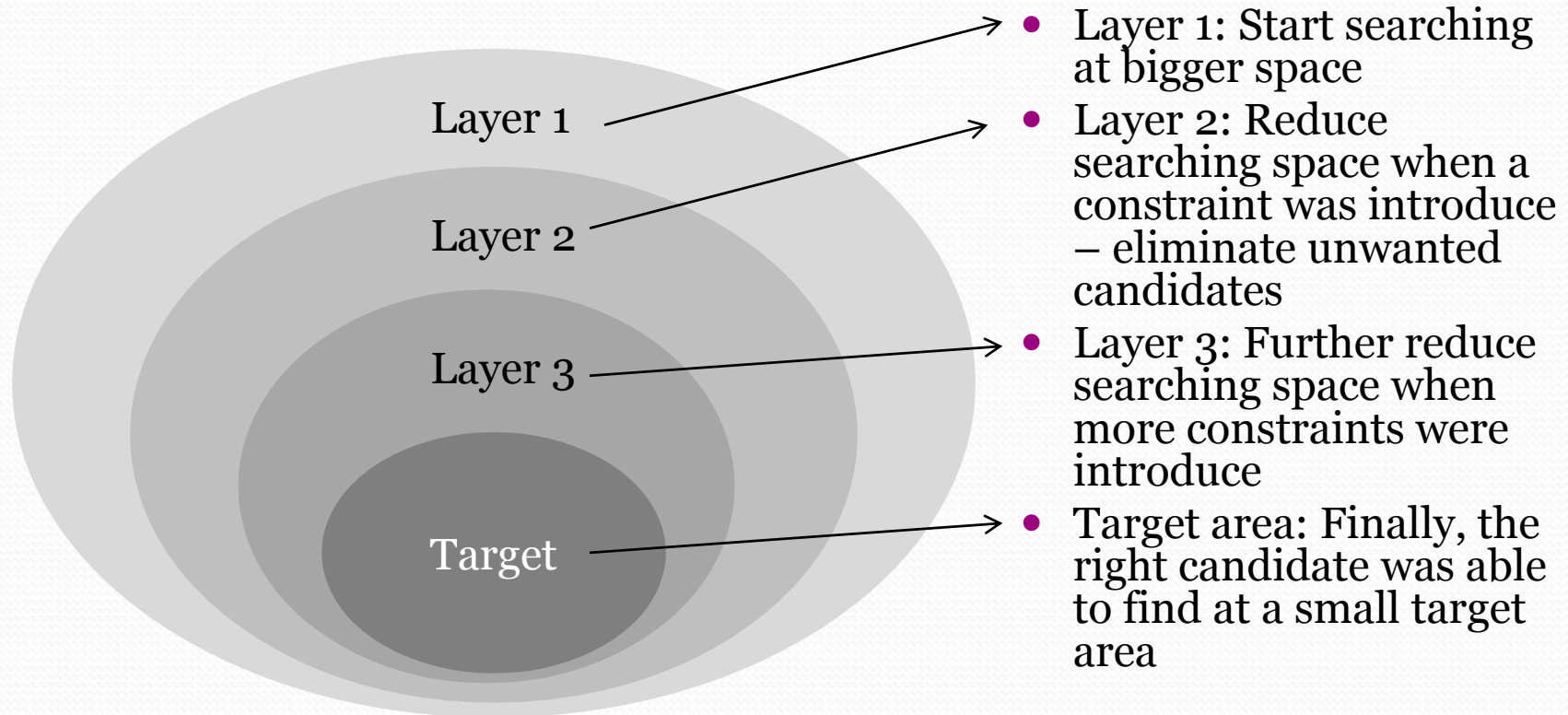
- Introduction
- Motivation
- Objective
- Methodology
- Results
- Future work

Introduction

Chemical Product Design



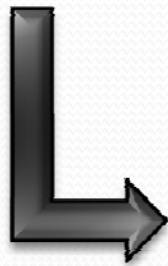
Introduction



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

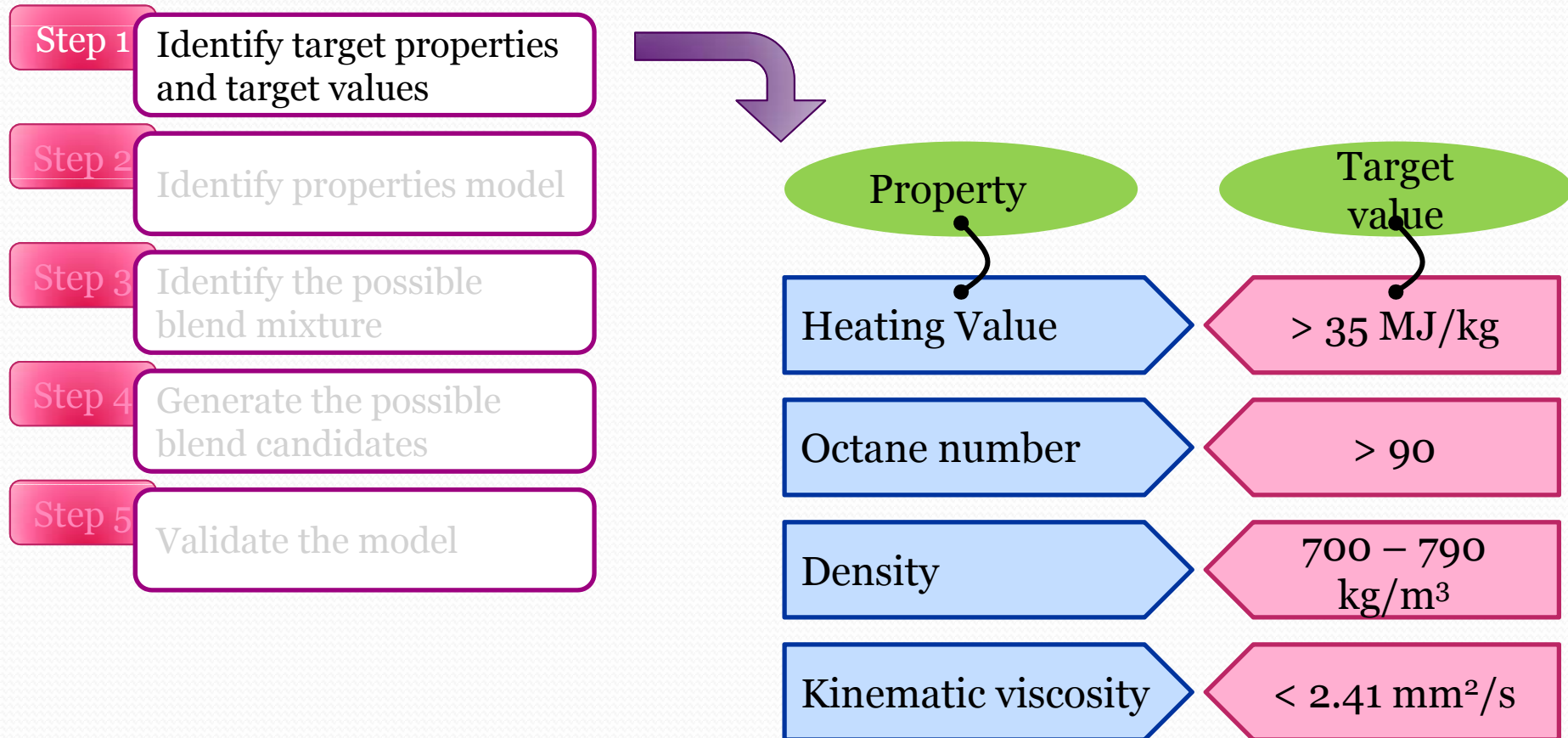
Validate the model

Methodology

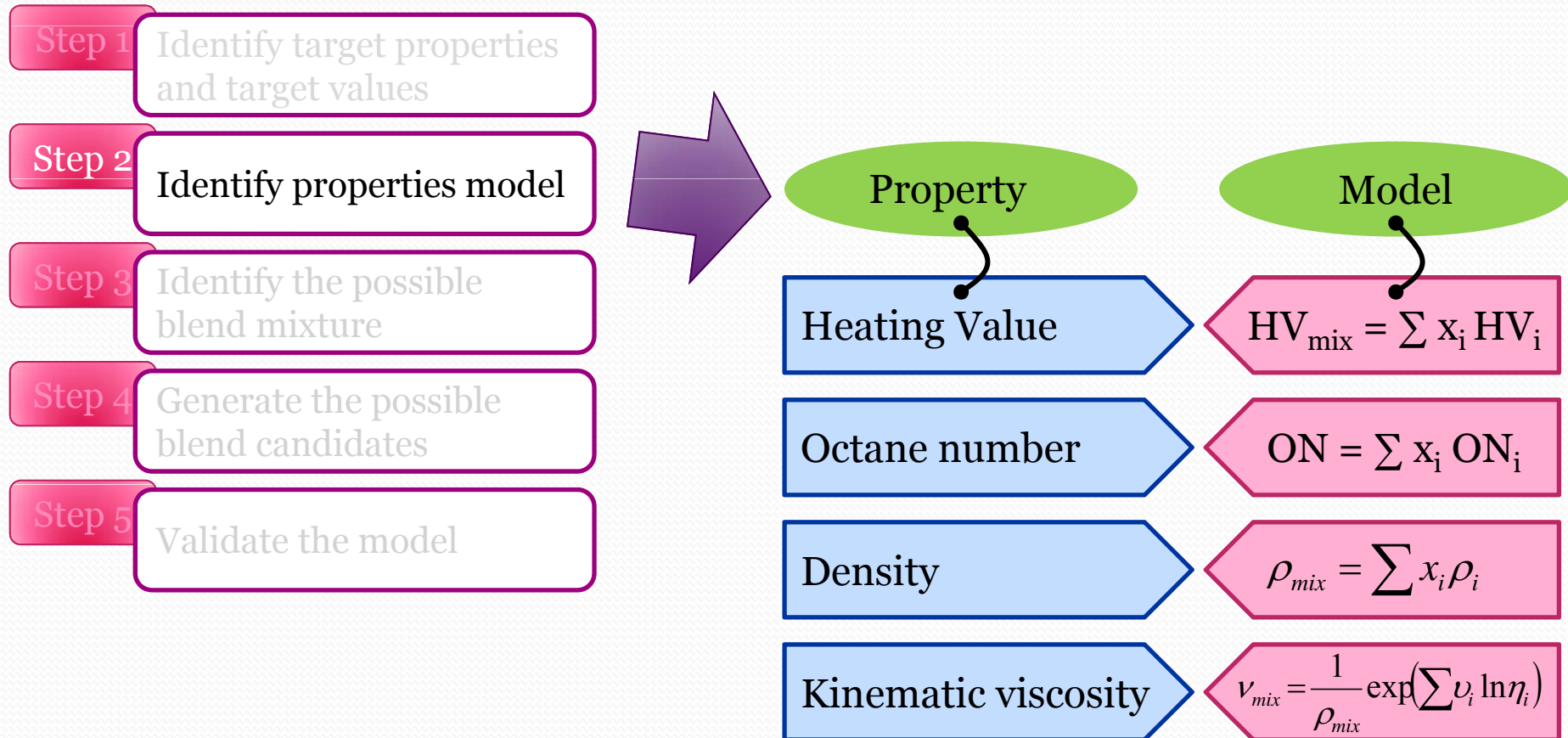
step	Task	Method & tools	Output
1	Identify the important target property	Literature (journals) Blending guideline	List of target properties
	Set the target value for each target property	Literature (journals), Blending regulation Existing product	List of constraints
2	Identify pure and mixture property 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

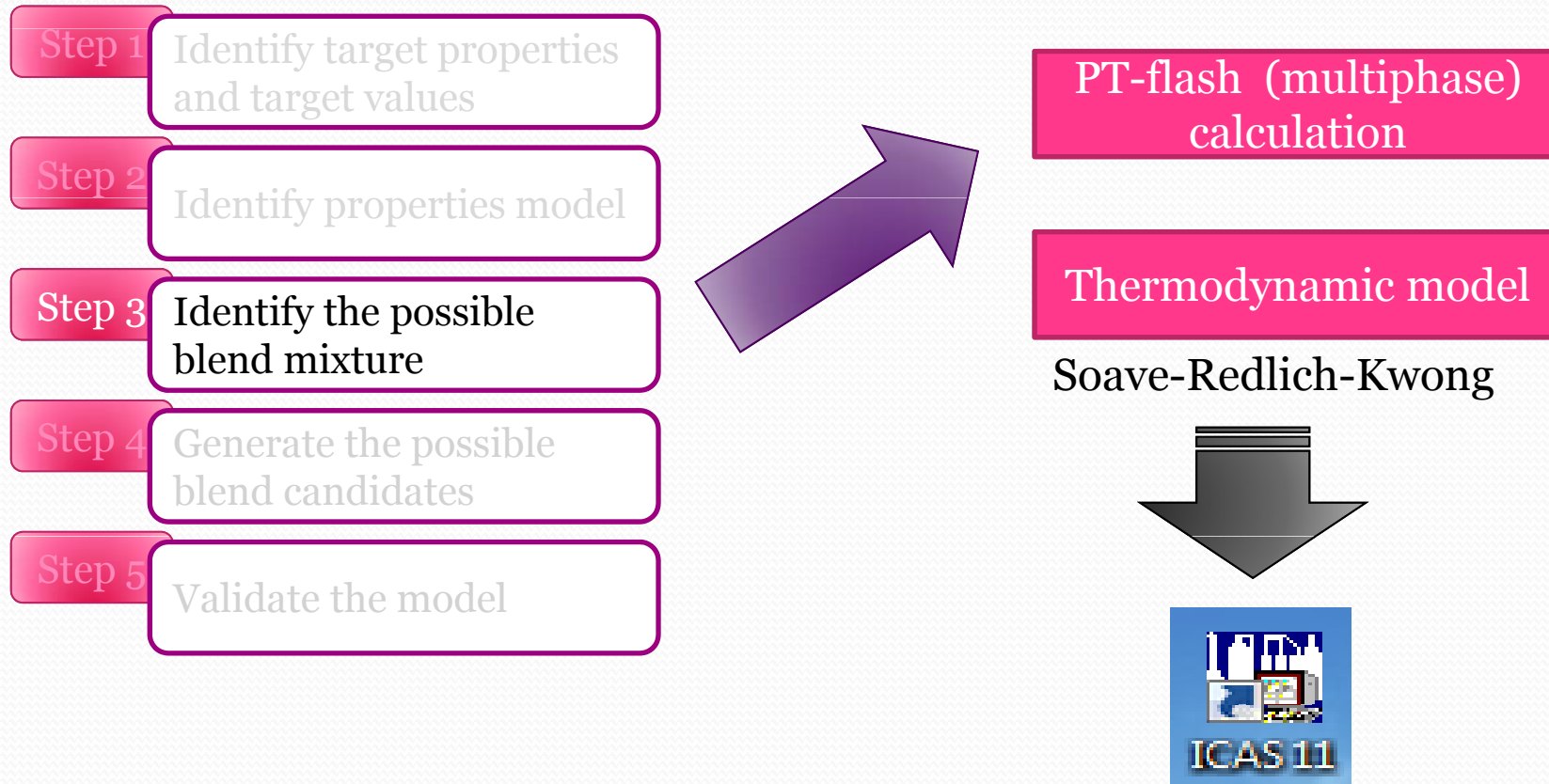
Methodology



Methodology



Methodology



Methodology

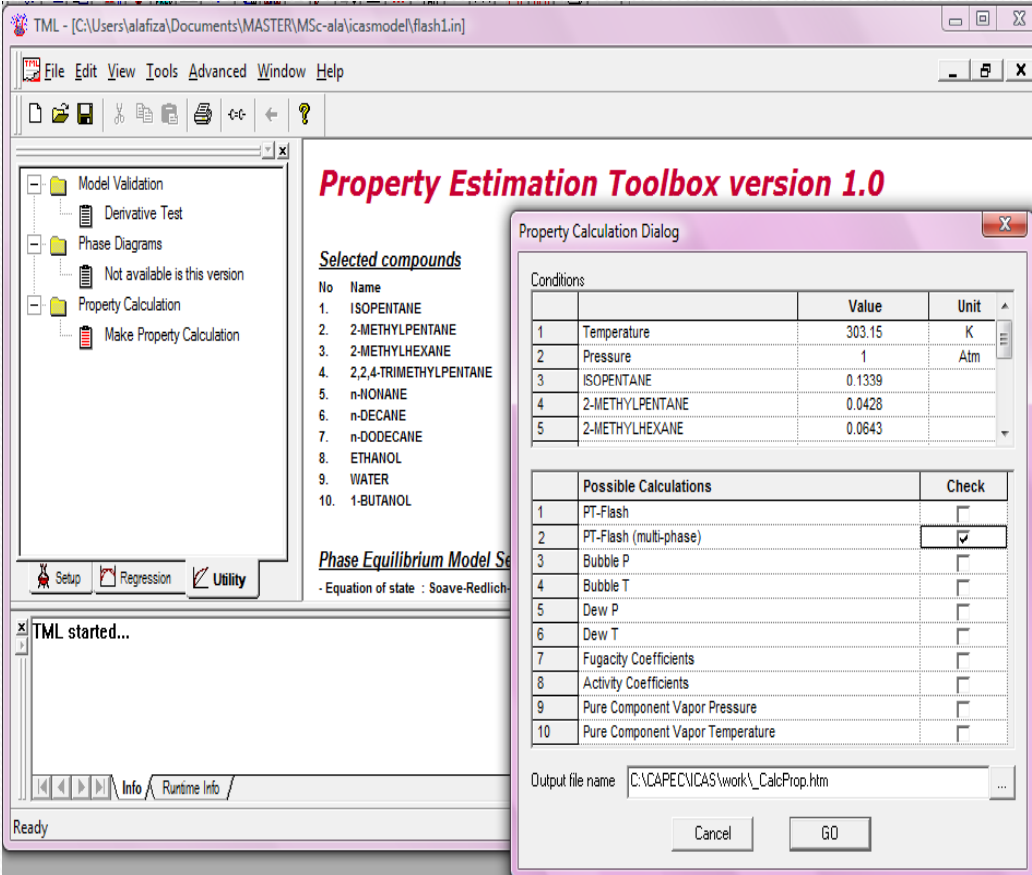
Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model



The screenshot displays the TML software interface. The main window shows a file explorer on the left with a tree view containing folders for Model Validation, Phase Diagrams, and Property Calculation. The main area displays the **Property Estimation Toolbox version 1.0** with a list of **Selected compounds**:

- ISOPENTANE
- 2-METHYLPENTANE
- 2-METHYLHEXANE
- 2,2,4-TRIMETHYLPENTANE
- n-NONANE
- n-DECANE
- n-DODECANE
- ETHANOL
- WATER
- 1-BUTANOL

The **Property Calculation Dialog** is open, showing the following conditions:

No	Name	Value	Unit
1	Temperature	303.15	K
2	Pressure	1	Atm
3	ISOPENTANE	0.1339	
4	2-METHYLPENTANE	0.0428	
5	2-METHYLHEXANE	0.0643	

Below the conditions table is a table for **Possible Calculations**:

No	Possible Calculations	Check
1	PT-Flash	<input type="checkbox"/>
2	PT-Flash (multi-phase)	<input checked="" type="checkbox"/>
3	Bubble P	<input type="checkbox"/>
4	Bubble T	<input type="checkbox"/>
5	Dew P	<input type="checkbox"/>
6	Dew T	<input type="checkbox"/>
7	Fugacity Coefficients	<input type="checkbox"/>
8	Activity Coefficients	<input type="checkbox"/>
9	Pure Component Vapor Pressure	<input type="checkbox"/>
10	Pure Component Vapor Temperature	<input type="checkbox"/>

The dialog also shows the **Output file name** as C:\CAPEC\ICAS\work\CalcProp.htm and buttons for **Cancel** and **GO**.

Methodology

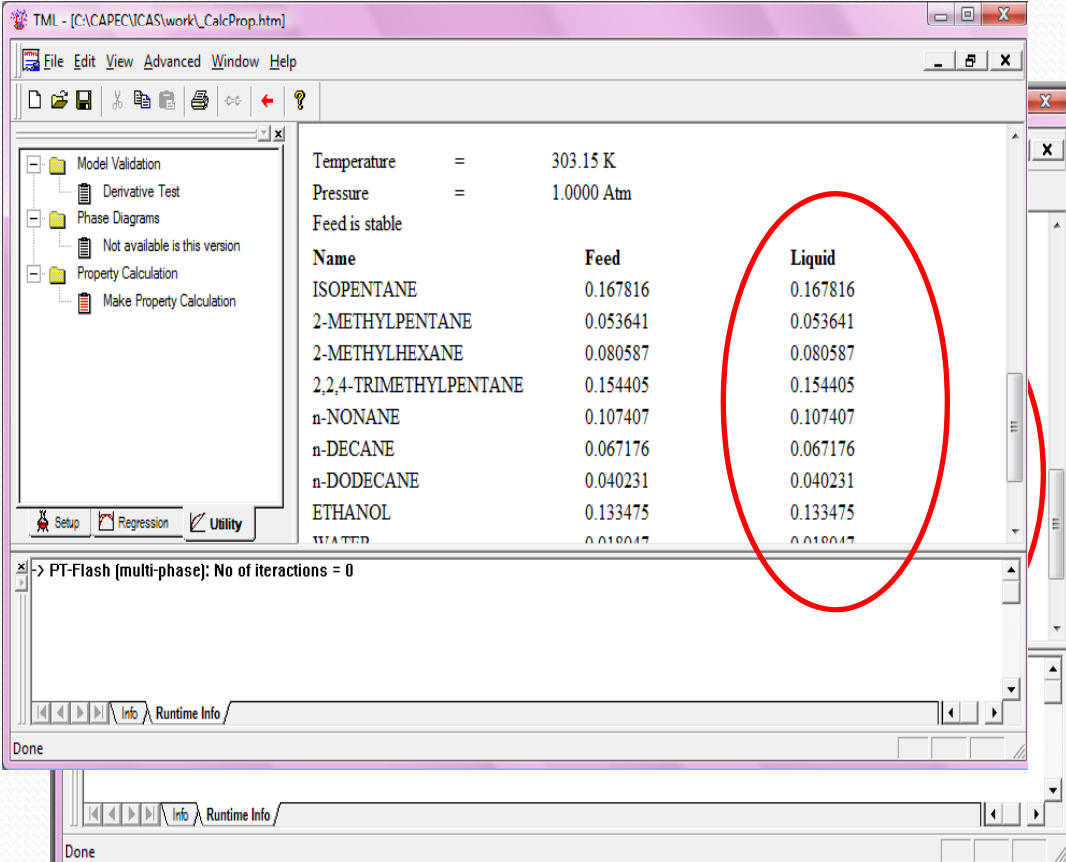
Step 1 Identify target properties and target values

Step 2 Identify properties model

Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model



TML - [C:\CAPEC\ICAS\work_CalcProp.htm]

File Edit View Advanced Window Help

Model Validation
Derivative Test
Phase Diagrams
Not available is this version
Property Calculation
Make Property Calculation

Temperature = 303.15 K
Pressure = 1.0000 Atm
Feed is stable

Name	Feed	Liquid
ISOPENTANE	0.167816	0.167816
2-METHYLPENTANE	0.053641	0.053641
2-METHYLHEXANE	0.080587	0.080587
2,2,4-TRIMETHYLPENTANE	0.154405	0.154405
n-NONANE	0.107407	0.107407
n-DECANE	0.067176	0.067176
n-DODECANE	0.040231	0.040231
ETHANOL	0.133475	0.133475
WATER	0.018047	0.018047

Setup Regression Utility

PT-Flash (multi-phase): No of iterations = 0

Info Runtime Info

Done

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:

$$HV = \sum x_i HV_i$$

$$ON = \sum x_i ON_i$$

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

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

Volume constraint

$$V_{gasoline} \geq 0.5$$

$$V_{ethanol} \leq 0.05$$

Methodology

Step 1 Identify target properties and target values

Step 2 Identify properties model

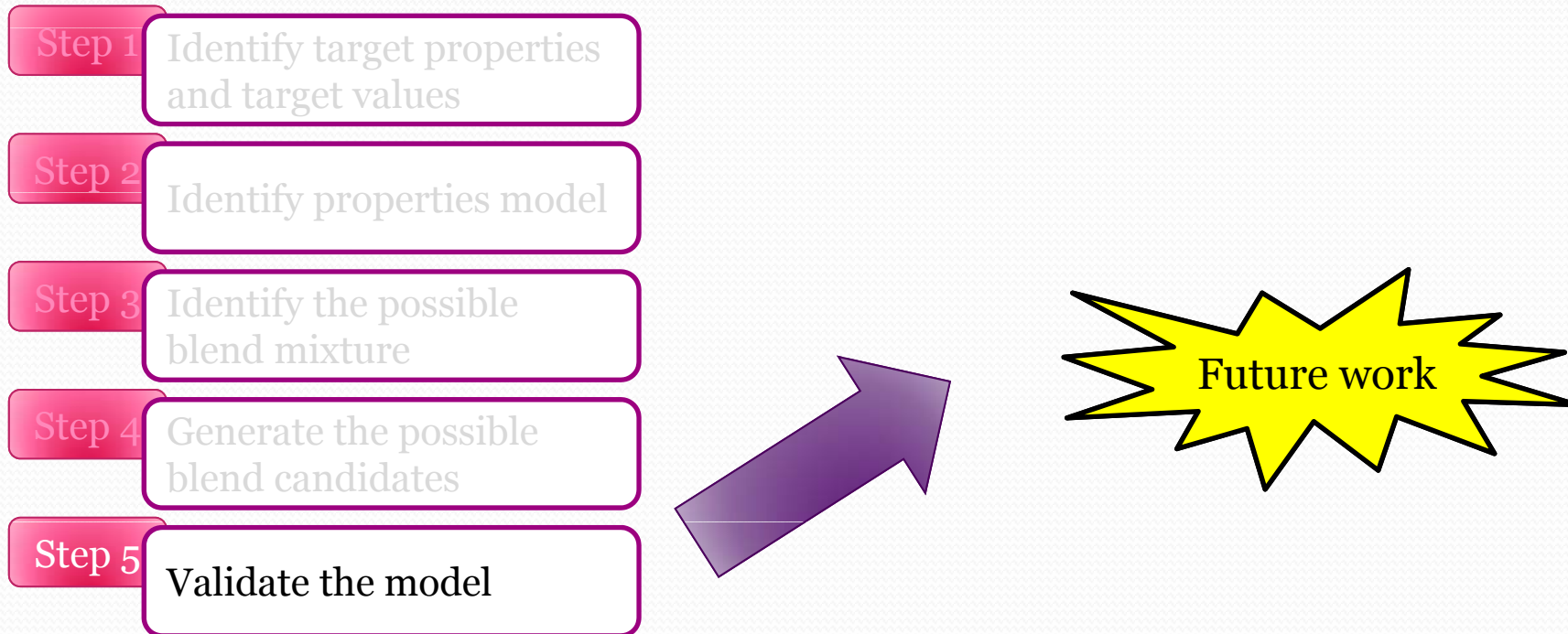
Step 3 Identify the possible blend mixture

Step 4 Generate the possible blend candidates

Step 5 Validate the model

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

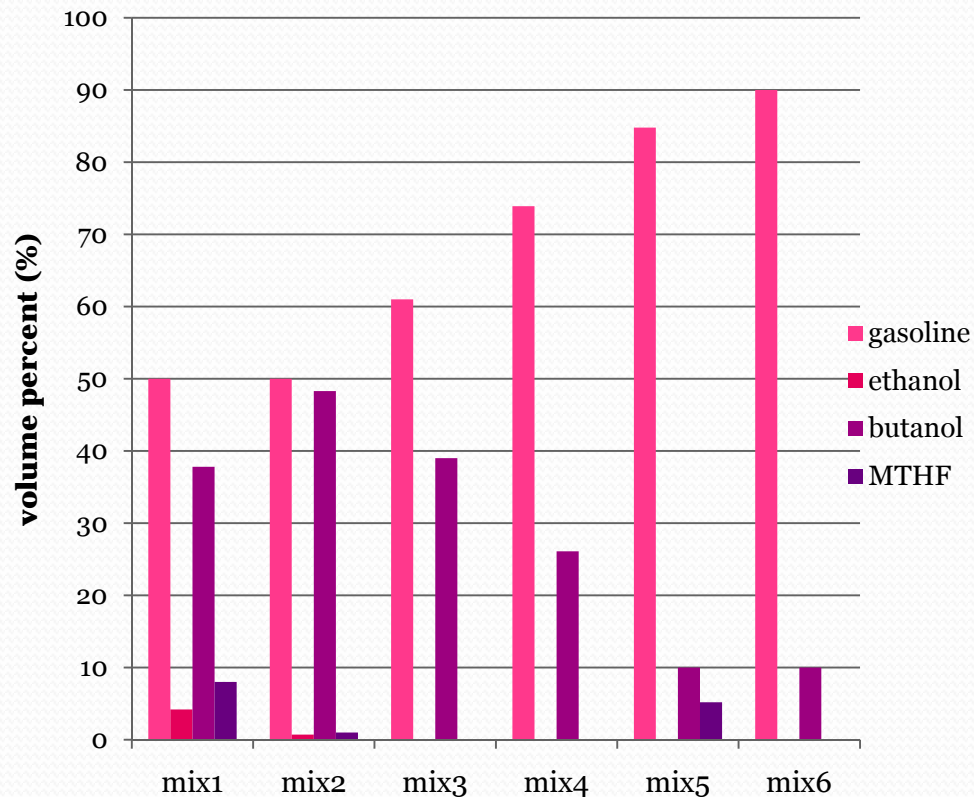
Methodology



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

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

Acknowledgment

- CAPEC, Technical University of Denmark, Denmark
- Universiti Teknologi Malaysia, Malaysia.

A wide-angle photograph of a vast field of yellow rapeseed flowers in full bloom. The flowers are densely packed and stretch towards a flat horizon under a clear, pale blue sky. The overall scene is bright and cheerful.

THANK YOU

Q&A session