RAPID
Transforming Process Industries

UNIVERSITY OF DELAWARE

Reaction Network Viewer (ReNView): An open-source framework for reaction path visualization of chemical reaction

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ReNView

Rapid Advancement in Process Intensification Deployment

AIChE
The Global Home of Chemical Engineers

About me

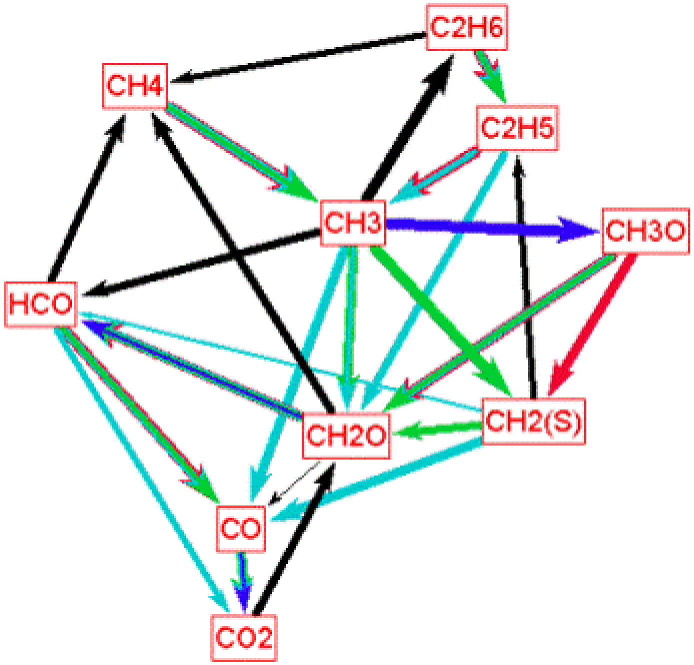
- Postdoctoral researcher from Vlachos group (May 2018 – Aug 2019)
- Solution Architect at Siemens Industry Software Inc.
- Based in Parsippany, New Jersey
- LinkedIn: https://www.linkedin.com/in/uditgupta0912/

Agenda

1. Reaction Network Viewer (RenView) slides
2. Demo session
3. Q&A

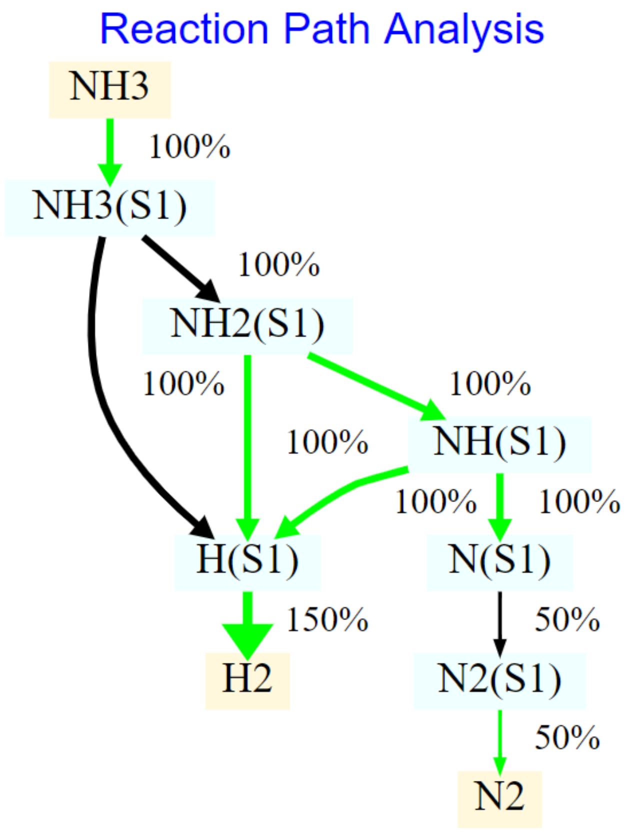
Reaction Path Visualizer (General Idea)

- Identify important species and reactions
- Identify equilibrated and fast reactions
- View the dominant chemistry in process
- Graphically explore chemical bottlenecks
- Key tool in mechanism reduction



[1]https://www.ansys.com/-/media/ansys/corporate/resourcelibrary/brochure/chemkin-pro-brochure.pdf

Reaction Path Visualizer



- **Green** edges represent equilibrated reactions
- **Black** edges represent surface reactions
- Reaction fluxes represented using edge thickness

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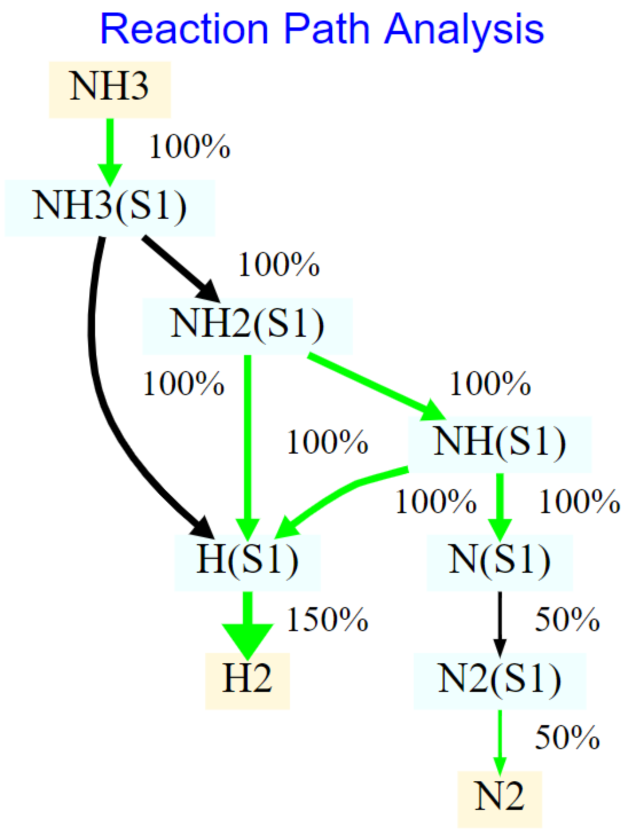

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  - Cutoff reaction rate – For edges
  - Visualization Elements – For nodes

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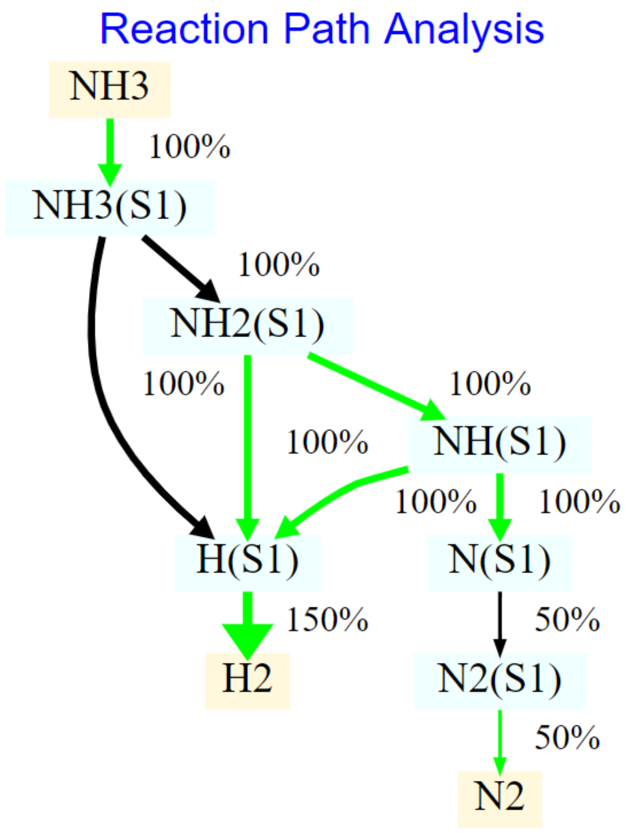

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  - Normalized using net rate of initial reactant
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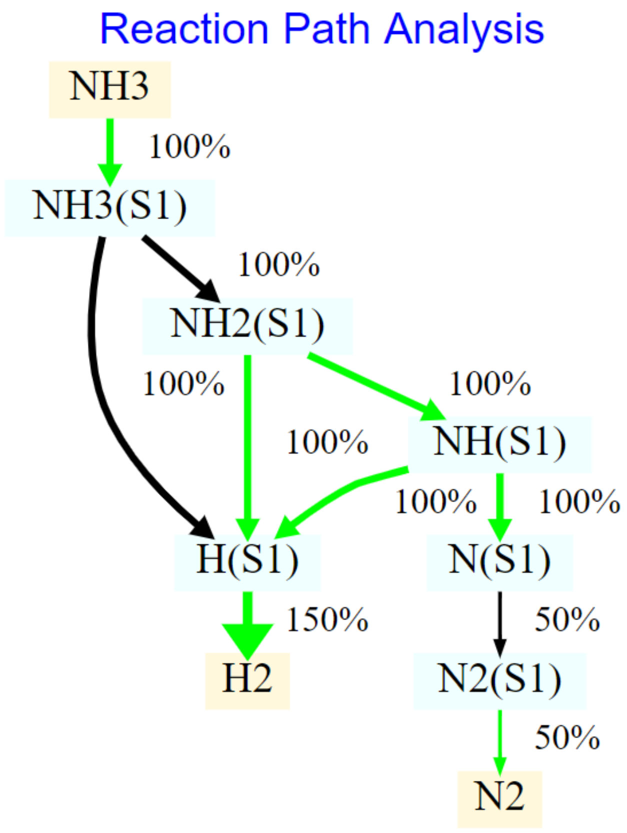

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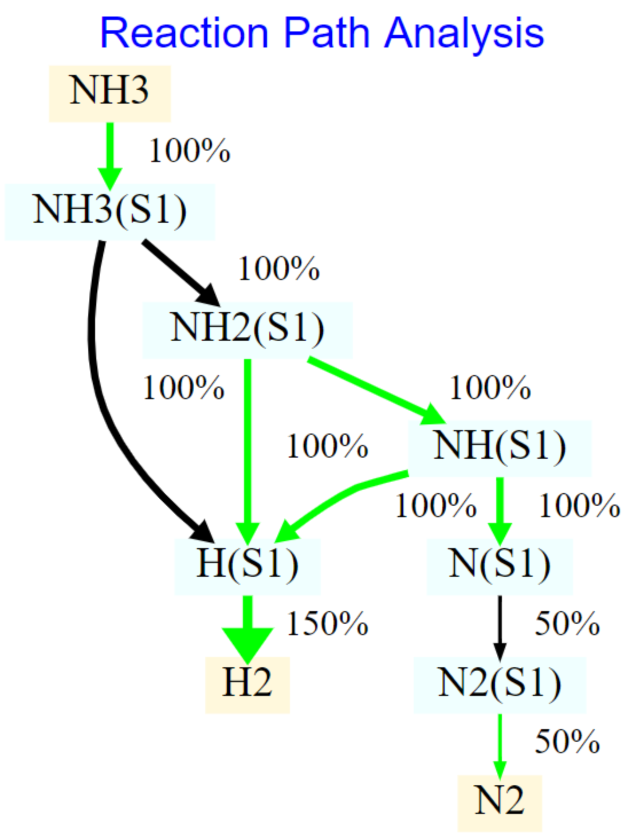

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- Generate at any point within the reactor

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Inputs to the visualizer

Fwd_Rate	Rev_Rate	Net_Rate	PEI	Reaction_String
4.99E-01	4.99E-01	-3.51E-08	5.00E-01	H2 + 2 RU(S1) <=> 2 H(S1) + 2 RU(B)
8.07E-02	8.07E-02	-1.17E-08	5.00E-01	N2 + RU(S1) <=> N2(S1) + RU(B)
5.49E-01	5.49E-01	2.34E-08	5.00E-01	NH3 + RU(S1) <=> NH3(S1) + RU(B)
2.50E-08	1.57E-09	2.34E-08	9.41E-01	NH3(S1) + RU(S1) <=> H(S1) + NH2(S1) + RU(B)
6.11E-06	6.09E-06	2.34E-08	5.01E-01	NH2(S1) + RU(S1) <=> H(S1) + NH(S1) + RU(B)
3.15E-04	3.15E-04	2.34E-08	5.00E-01	NH(S1) + RU(S1) <=> H(S1) + N(S1) + RU(B)
6.93E-14	1.17E-08	-1.17E-08	5.92E-06	N2(S1) + RU(S1) <=> 2 N(S1) + RU(B)

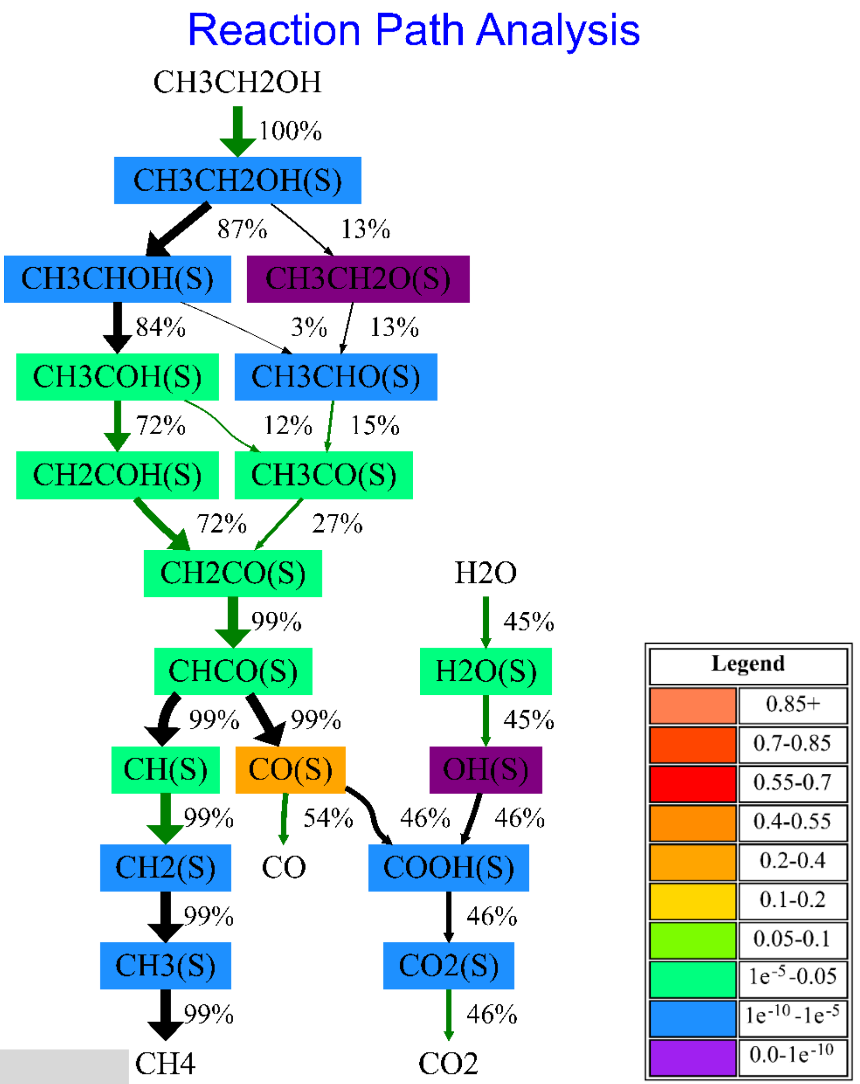
Reactions file

Species_name	Phase	N	H	RU
H2	Gas	0	2	0
N2	Gas	2	0	0
NH3	Gas	1	3	0
RU(B)	Surface	0	0	1
RU(S1)	Surface	0	0	1
N2(S1)	Surface	2	0	0
N(S1)	Surface	1	0	0
H(S1)	Surface	0	1	0
NH3(S1)	Surface	1	3	0
NH2(S1)	Surface	1	2	0
NH(S1)	Surface	1	1	0

Species file

- Input files contain species and reaction flux information
- **No need for inputs if connected to kinetic simulator** since we already have the set of reactions specified and fluxes from simulation.

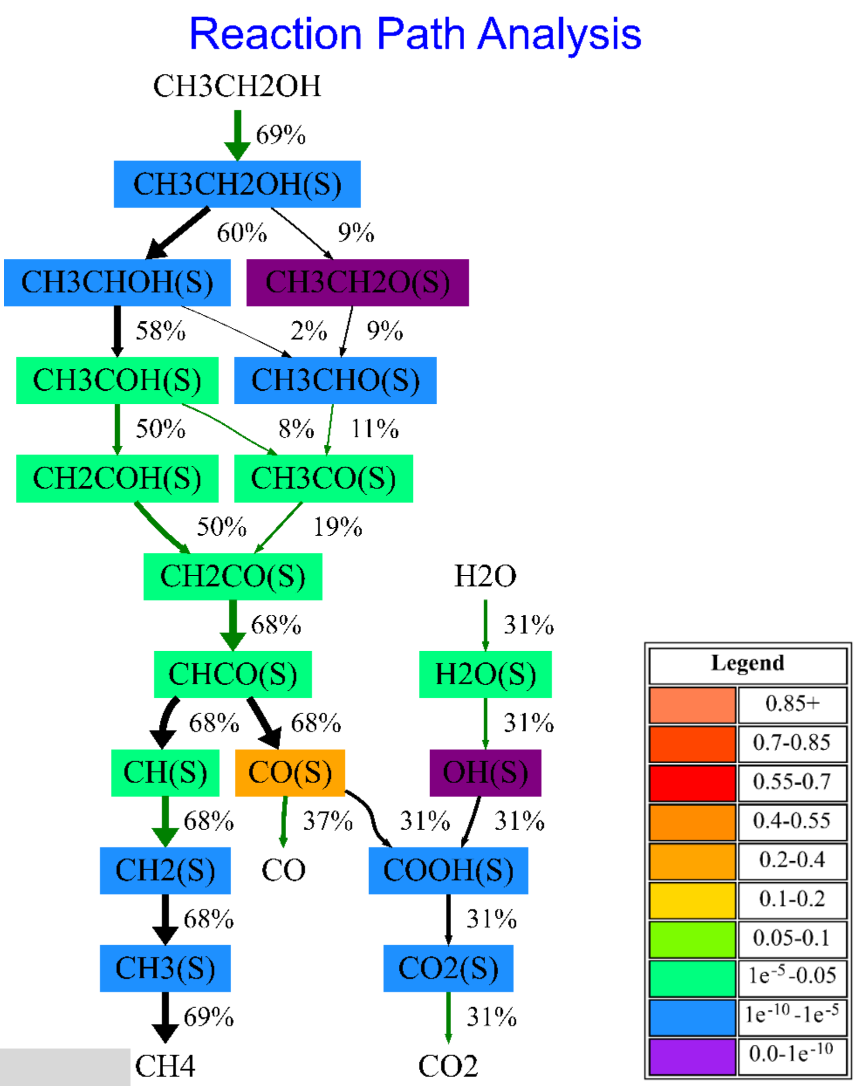
Normalized using net rate of inlet reactant



$$Edge\ label, e_i = \frac{Reaction\ rate, r_i}{\sum_{j=1}^{n} r_j} * 100$$

- Generally seen in homogeneous systems like combustion, pyrolysis
- One mole of ethanol yields one mole of methane, 0.54 moles of CO, and 0.46 moles of CO_2

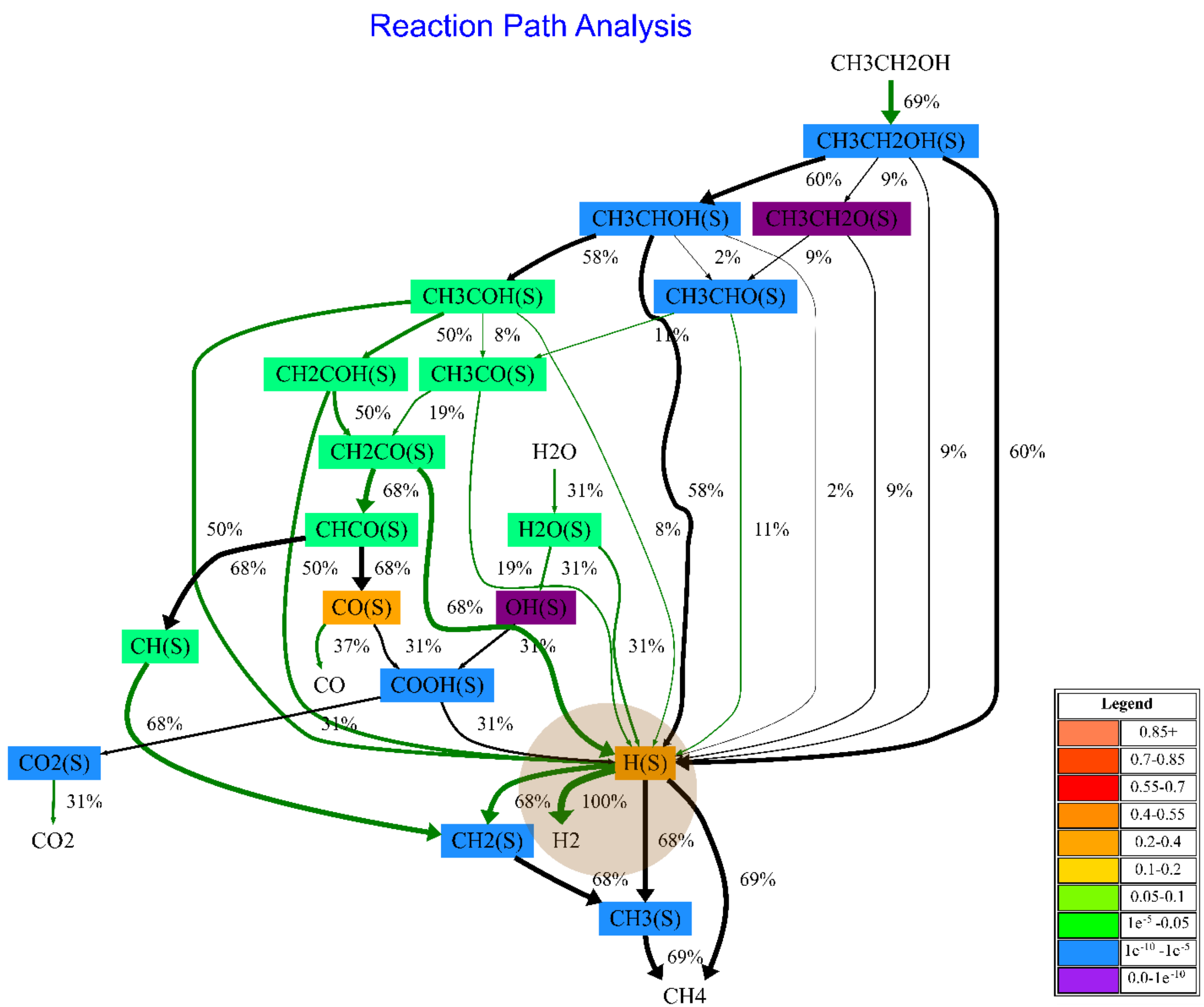
Normalized using maximum rate in the network



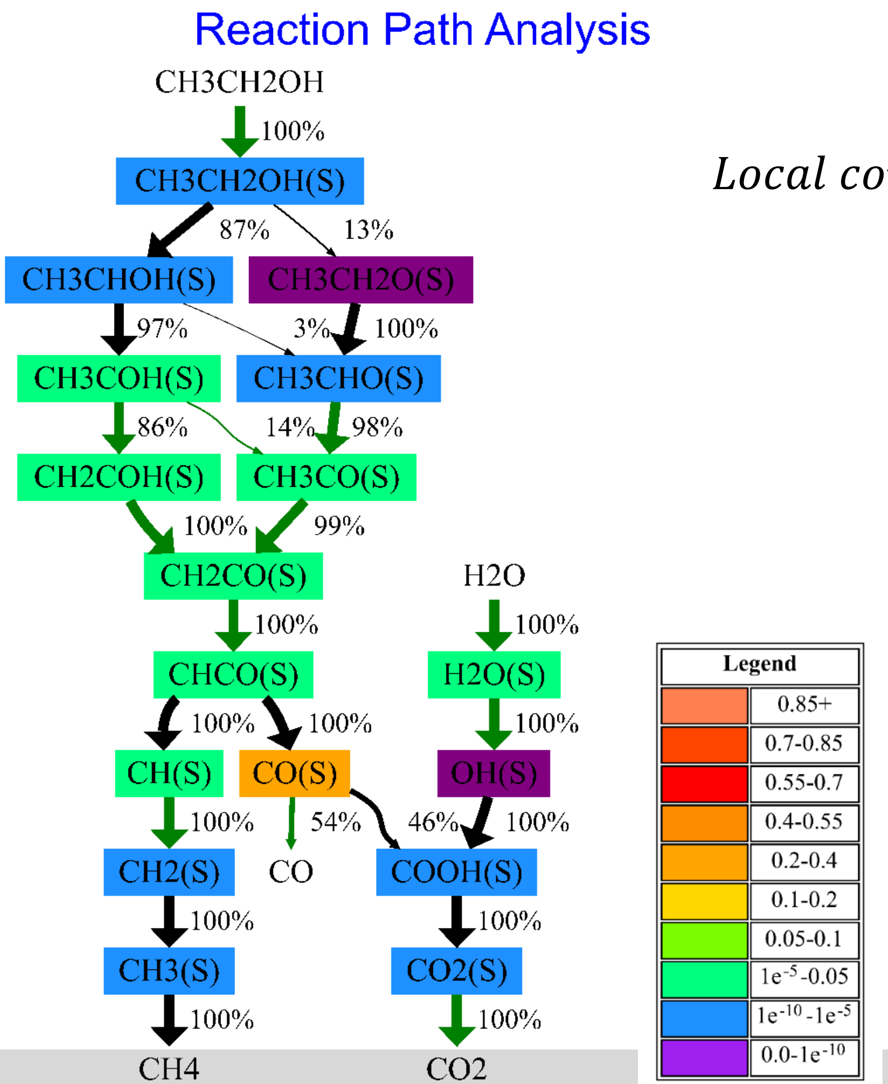
$$Edge\ label, e_i = \frac{Reaction\ rate, r_i}{r_{\max rate}} * 100$$

- Useful for heterogeneous reaction systems where reaction flux is dependent on surface coverage of intermediate
- Maximum reaction rate provides an upper bound on flux
- Node colors represent surface coverages

Normalized using maximum rate in the network



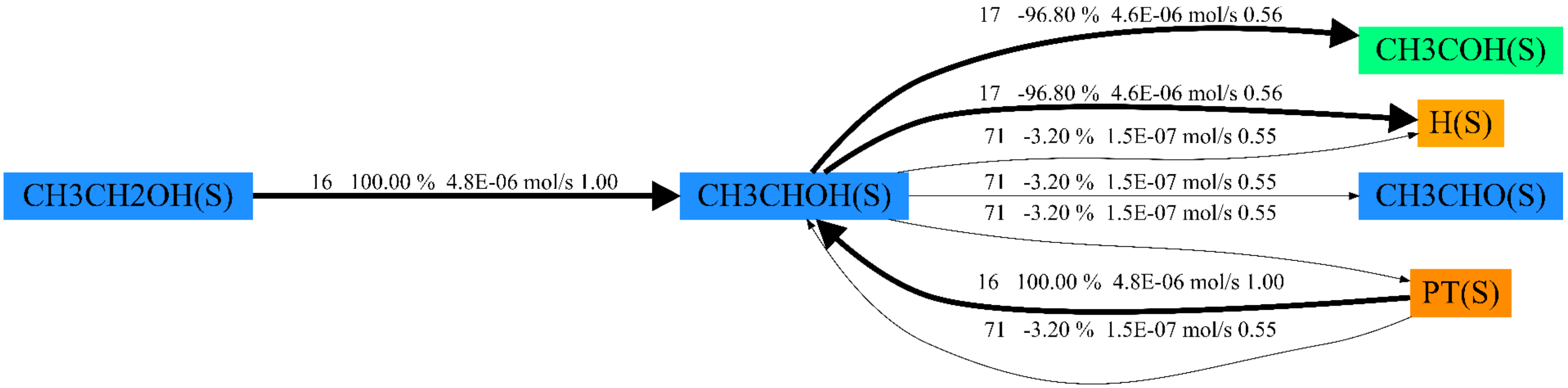
Common basis 100% (local consumption)



$$Local\ consumption\ of\ reaction\ r_{i,S} = \frac{r_i}{\sum_{j=1}^{m} r_j} * 100$$

Provides local analysis of reaction fluxes

Species Visualization



For **non-equilibrium** reactions, we specify the following details:
1. Reaction Number
2. % Prod/Cons for the specific reaction
3. Net-rate of the reaction
4. Partial Equilibrium Index (pei)

For **equilibrated** reactions, we specify the following details:
1. Reaction Number
2. % Prod/Cons for the specific reaction
3. Equilibrium constant for the specific reaction (with units)
4. Partial Equilibrium Index (pei)

Case Studies

	Species	Reactions
Ammonia synthesis	11	7
Ethanol reforming on Pt	68	162
p-cresol hydrodeoxygenation (HDO)	183	500

GitHub: https://github.com/VlachosGroup/ReNView

Documentation: https://github.com/VlachosGroup/renview/wiki/Documentation

Citation: U. Gupta and D. G. Vlachos, SoftwareX, 2020. 11: p. 100442
https://www.sciencedirect.com/science/article/pii/S2352711019302432

Future Work

- Preliminary work done on listing the **dominant pathways** in the visualization
- The output will generate the top 5 pathways (if present) from Species A to B based on users' input
- **Rate-determining steps** will also be identified for each pathway
- **Graphical user interface** for easier usability

Hands-on Exercises

Ammonia synthesis

Input specifications	
Species file	/data/example_ammonia/species_comp.out
Reactions file	/data/example_ammonia/reaction_rates.out
Initial reactant	NH3
Reaction cutoff rate	1.0E-09
Elements desired	'N', 'H'
Normalization	1 or 2 or 3
Output directory	/results/example_ammonia/

Ethanol steam reforming on Pt

Input specifications	
Species file	/data/example_sutton/species_comp.out
Reactions file	/data/example_sutton/reaction_rates.out
Initial reactant	CH3CH2OH
Reaction cutoff rate	1.0E-07
Elements desired	'C', 'O', 'H'
Normalization	1 or 2 or 3
Output directory	/results/example_sutton/

p-cresol hydrodeoxygenation (HDO)

Input specifications	
Species file	/data/example_gu_long_contact_time/species_comp.out
Reactions file	/data/example_gu_long_contact_time/reaction_rates.out
Initial reactant	PCOH
Reaction cutoff rate	1.0E-08
Elements desired	'C'
Normalization	1 or 2 or 3
Output directory	/results/example_gu_long_contact_time/

Questions?