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How to Use Your Process Simulator for Flammability Control

Rocky Costello, P.E. will demonstrate how to utilize process simulation to understand flammability risks, enhancing your safety measures and protecting your operations.

Meet the Presenter

Chemstations Partner

Rocky Costello

Chemical Engineer with 25+ years of experience in the chemical process industries and hazardous waste.

Rocky founded R. C. COSTELLO & ASSOC., Inc. to support the chemical engineering industry with innovative chemical and environmental engineering services, advanced and emerging process technologies, and regulatory compliance support.

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GROUP POLL

When work challenges cannot be solved with my current software . . .

A. I look for new software with built-in functionality.

B. Someone on my team can implement a custom solution.

C. I seek outside services such as consulting.

Introduction

What is Flammability?

A material is **flammable** if it ignites easily at ambient temperatures. A hydrocarbon mixture cannot ignite if there is not a flammable mixture of hydrocarbons and oxygen and an ignition source

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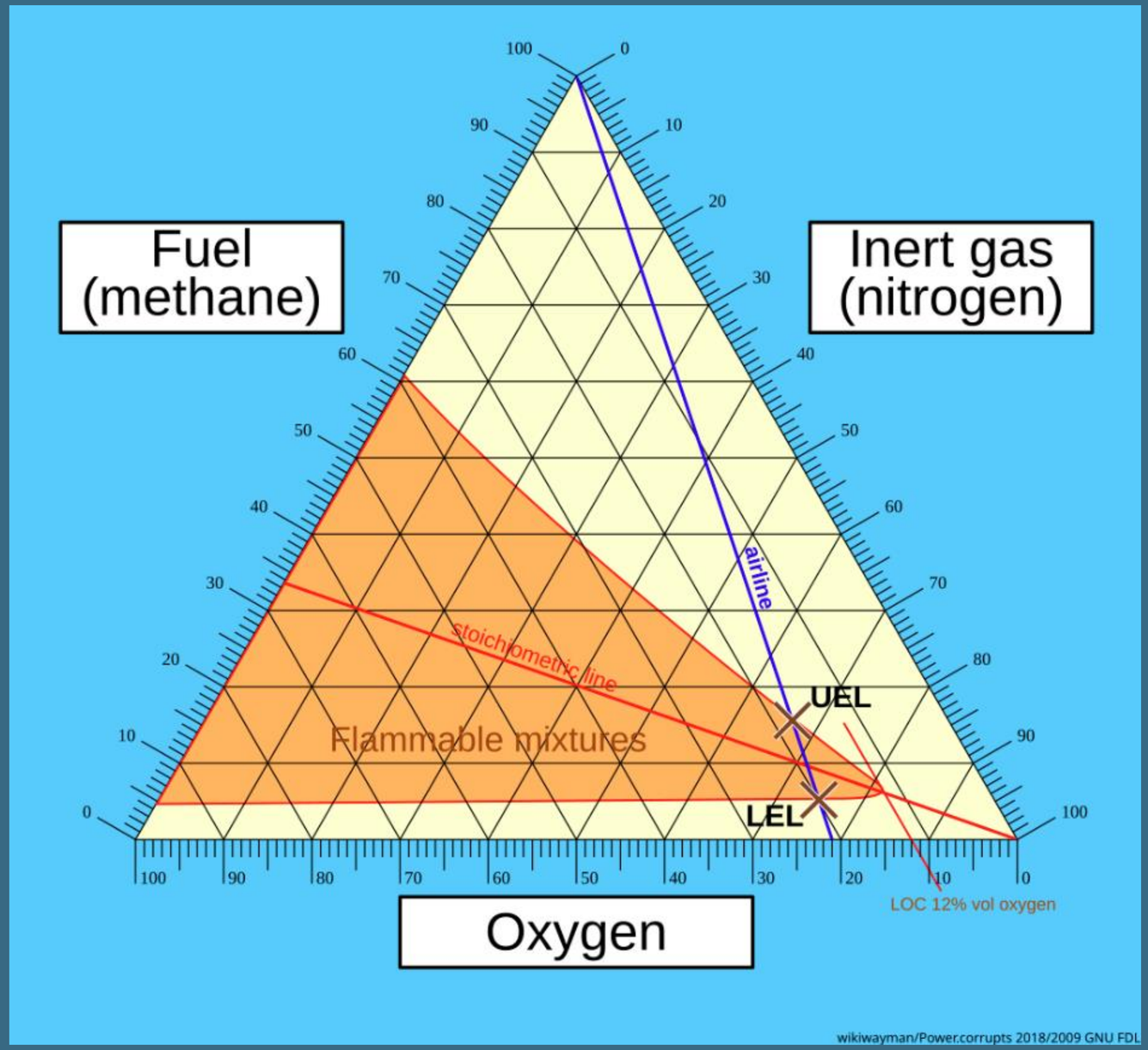
What is Flammability?

- Each individual hydrocarbon has both upper and lower flammability limits (UFL and LFL).
- A mixture of hydrocarbons also has a LFL and UFL, but this must be calculated using mole percents of the hydrocarbons in the vapor stream.
- A minimum level of oxygen is also necessary for combustion.

METHANE FLAMMABILITY DIAGRAM



Flammability diagram. Wikipedia, The Free Encyclopedia. May 21, 2024, 02:21 UTC. Available at: https://en.wikipedia.org/w/index.php?title=Flammability_diagram&oldid=1224888600.

A flammability diagram is a very useful tool for determining whether or not a hydrocarbon / oxygen mixture is flammable.

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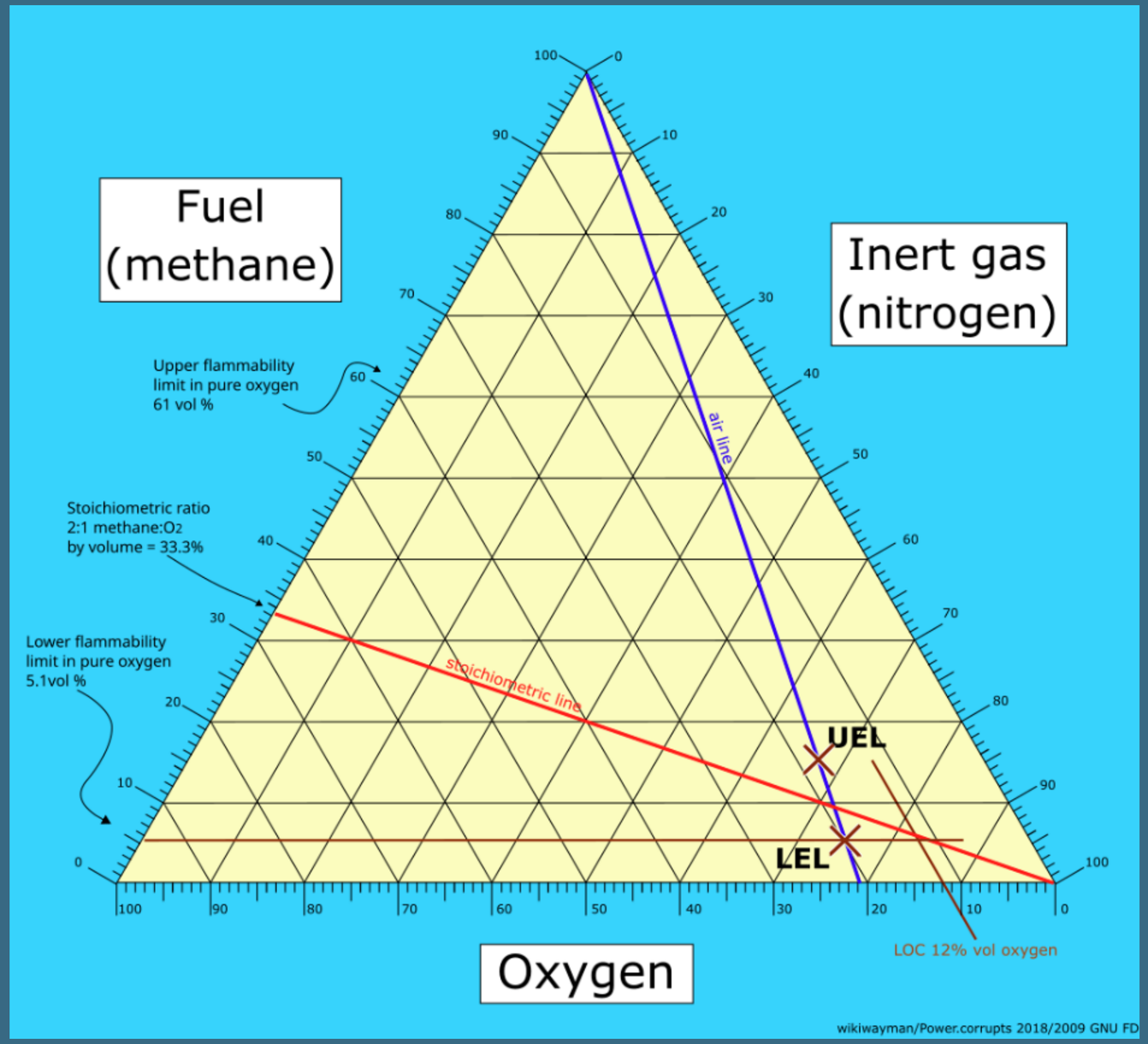
METHANE FLAMMABILITY DIAGRAM



Flammability diagram. Wikipedia, The Free Encyclopedia. May 21, 2024, 02:21 UTC. Available at: https://en.wikipedia.org/w/index.php?title=Flammability_diagram&oldid=1224888600.

The flammability is bound by the:

- LFL-UFL line
- LFL- MOC line
- UFL-MOC line

Where the stoichiometric line meets the LFL-UFL line is where maximum deflagration pressure is reached during an ignition. This is typically 10x the initial pressure.

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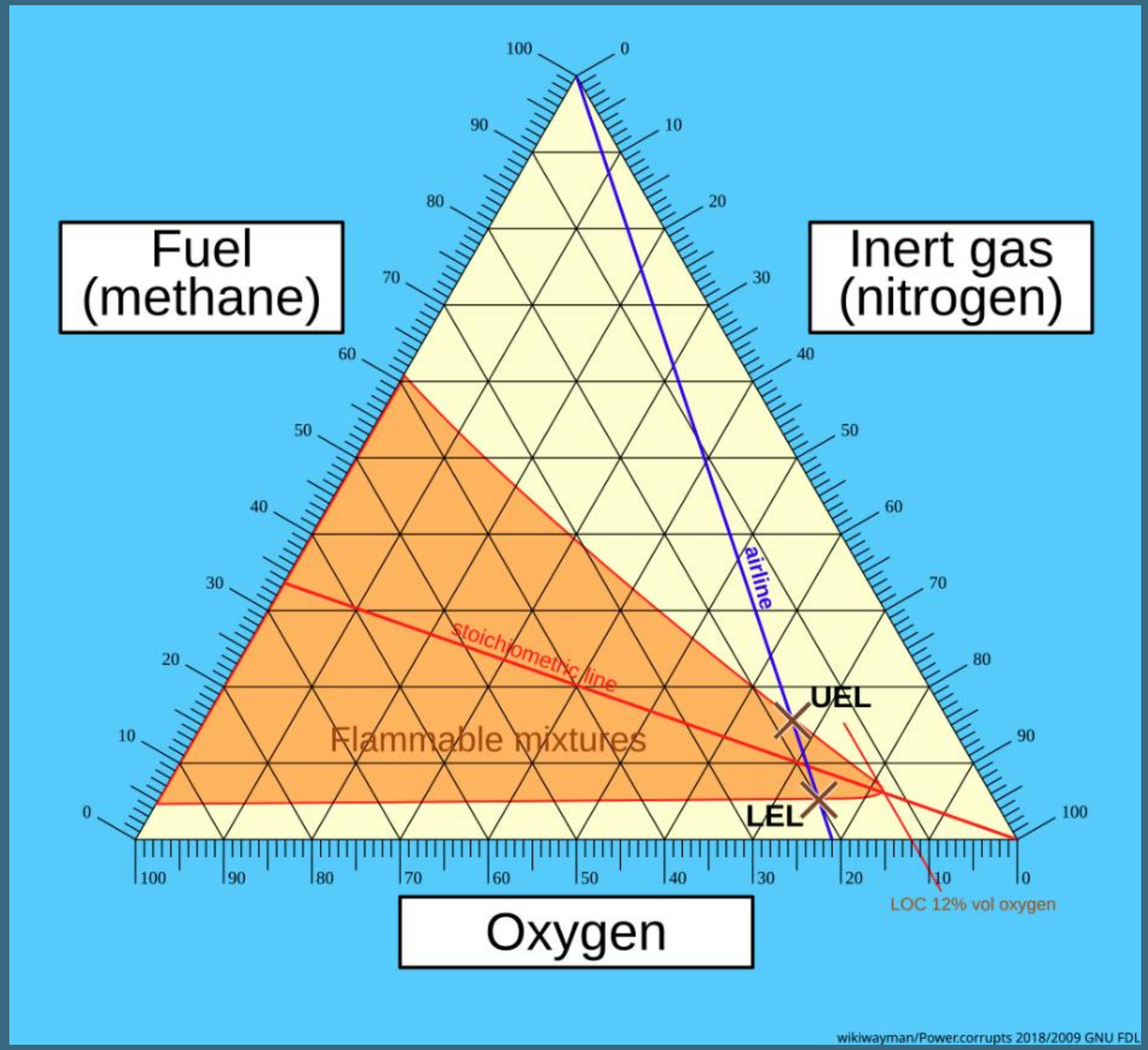
METHANE FLAMMABILITY DIAGRAM



Flammability diagram. Wikipedia, The Free Encyclopedia. May 21, 2024, 02:21 UTC. Available at: https://en.wikipedia.org/w/index.php?title=Flammability_diagram&oldid=1224888600.

As you move down the stoichiometric line and reach the MOC, the pressure multiplier is zero.

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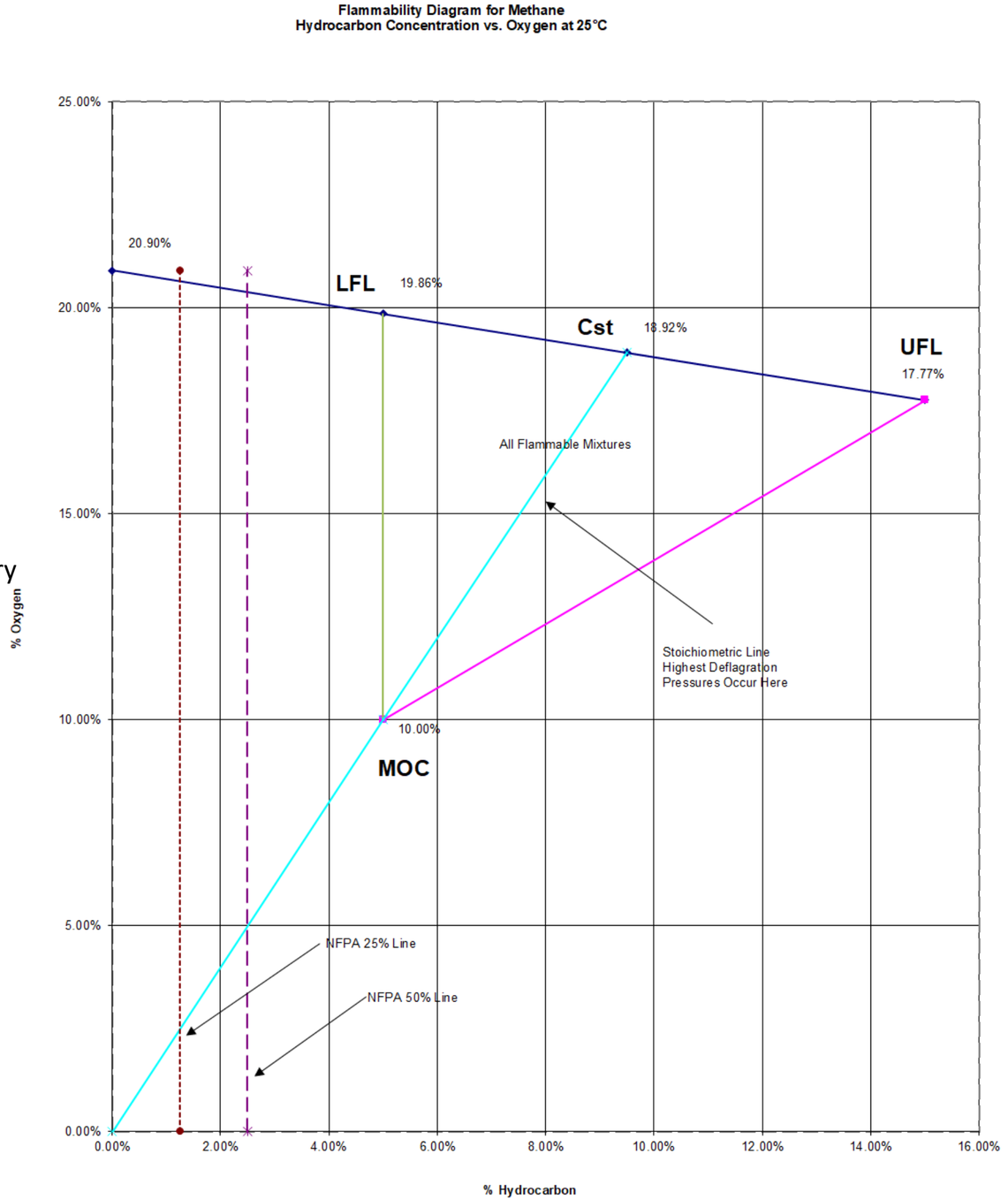
Let’s switch to Cartesian coordinates

Here is a Flammability diagram for the pure compound methane.

Inerts are determined by 100% - O2% - HC%

Cartesian Coordinates are easier to work with than Tertiary diagrams.

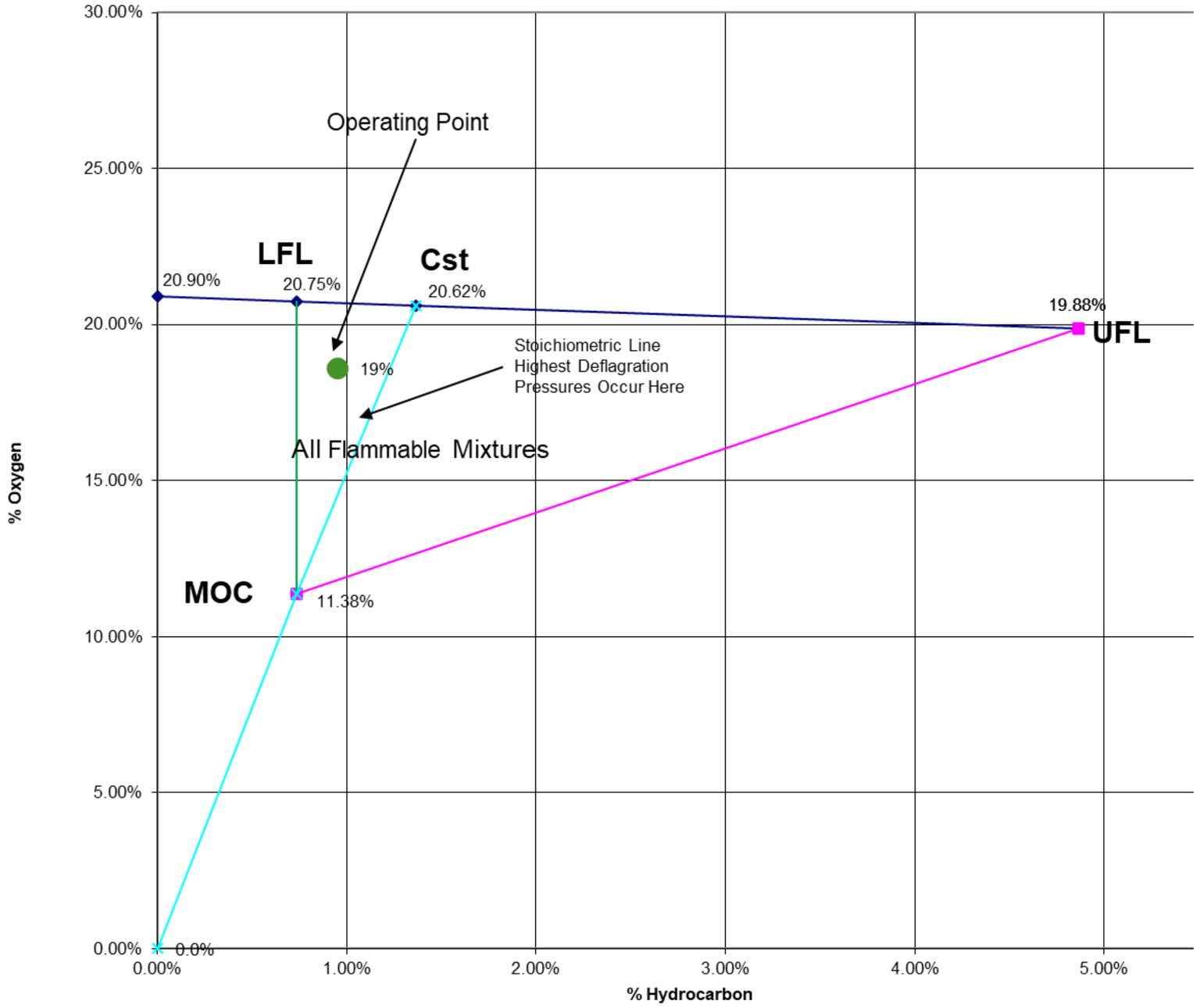


Calculation Methods

- The calculation method was originally prepared by the bureau of mines in 1947. It now can be found in Industrial Explosion Prevention and Protection by Frank Bodurtha.
- Composite LFL, UFL and MOCs are calculated within the spread sheet based on known values for the individual compounds using:

$$LFL_{mix} = 1/\sum_{i=1}^{n}(y_i/LFLi), \qquad UFL_{mix} = 1/\sum_{i=1}^{n}(y_i/UFLi)$$

- If the LFL, UFL and MOC values are not found in literature then the spreadsheet calculates them.
- Temperature correction is also included as the envelope opens up at higher temperatures
  - LFL decreases as T goes up by about 8% per every 100°C
  - UFL Increases as T goes up by about 8% per every 100°C
- Pressure correction is also included as the envelope _____ at higher pressures
  - LFL has slight change as P goes up
  - UFL greatly increases as P goes up



COMPOSITE FLAMMABILITY DIAGRAM

for Asphalt Vapors

LFL – Lower flammability limit

UFL – Upper flammability limit

MOC – minimum oxygen of combustion

Cst – Stoichiometric line of combustion

All operating points inside the flammable envelope represent flammable mixtures.

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GROUP POLL

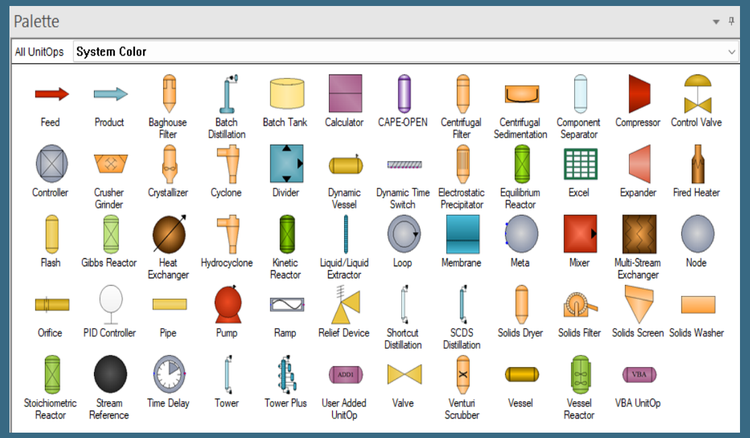
Is process simulation part of your work?

A. Yes, I use a process simulator but not CHEMCAD.

B. Yes, and I use CHEMCAD.

C. No, I don’t use a process simulator.

CHEMCADNXT



CHEMCAD is process simulation software that helps engineers achieve cost savings, improved safety, and operational efficiency.

CHEMCAD Process Simulator

Built-in Features	Chemicals (2K+), thermodynamics, equipment, etc.
Intuitive Interface	Design & test in a virtual environment
Customizable	Integrate code for specialized functionality

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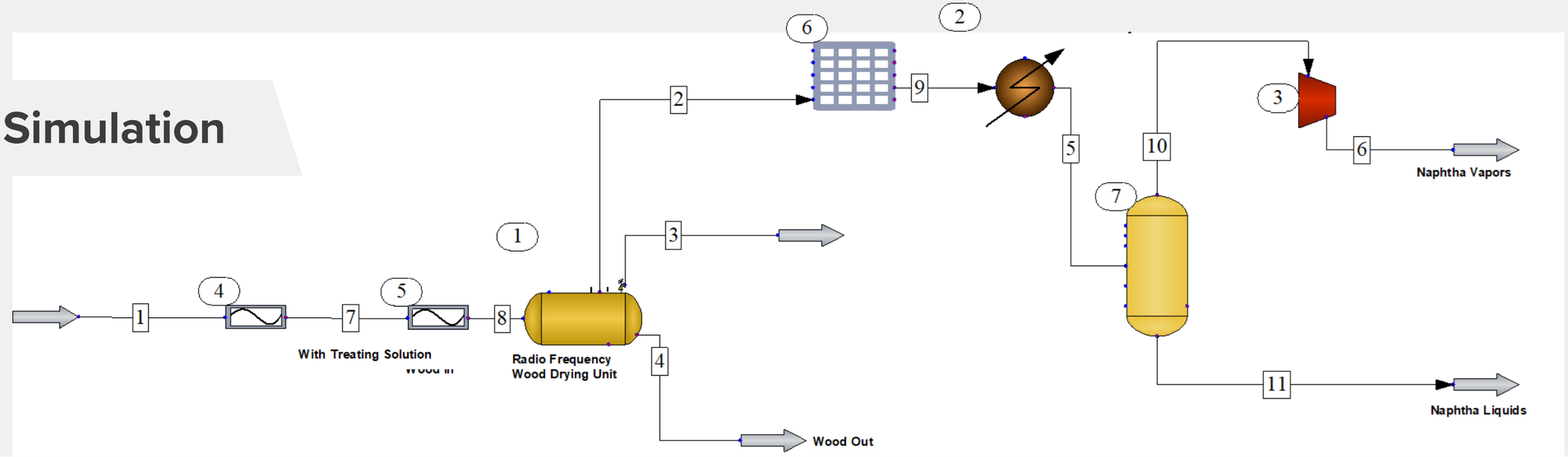
CHEMCADNXT

Process Simulator & Flammability Diagram

- An Excel unit operation with a flammability diagram can be used to determine whether a mixture lies in the flammable envelope.
- The following simulation is a dynamic simulation of a wood drying operation where a solvent laden with a pesticide is absorbed into the wood.
- Using the Excel unit operation in conjunction with a flammability worksheet, it can be determined whether or not the drying operation can be conducted safely.

Simulation



- The flowsheet represents a dynamic simulation of a wood drying operation.
- Hydrocarbon solution with a pesticide for termites is applied to the wood where the wood is soaked, pressurized to push the solution into the wood and finally drained.
- The dynamic vessel represents this vessel an autoclave.
- Ramp functions change the pressure from atmospheric to 2 psia, and add heat.
- The excel unit operation interfaces with the flammability diagram.
- The hydrocarbons are condensed and collected. The compressor unit operation represents the vacuum pump.

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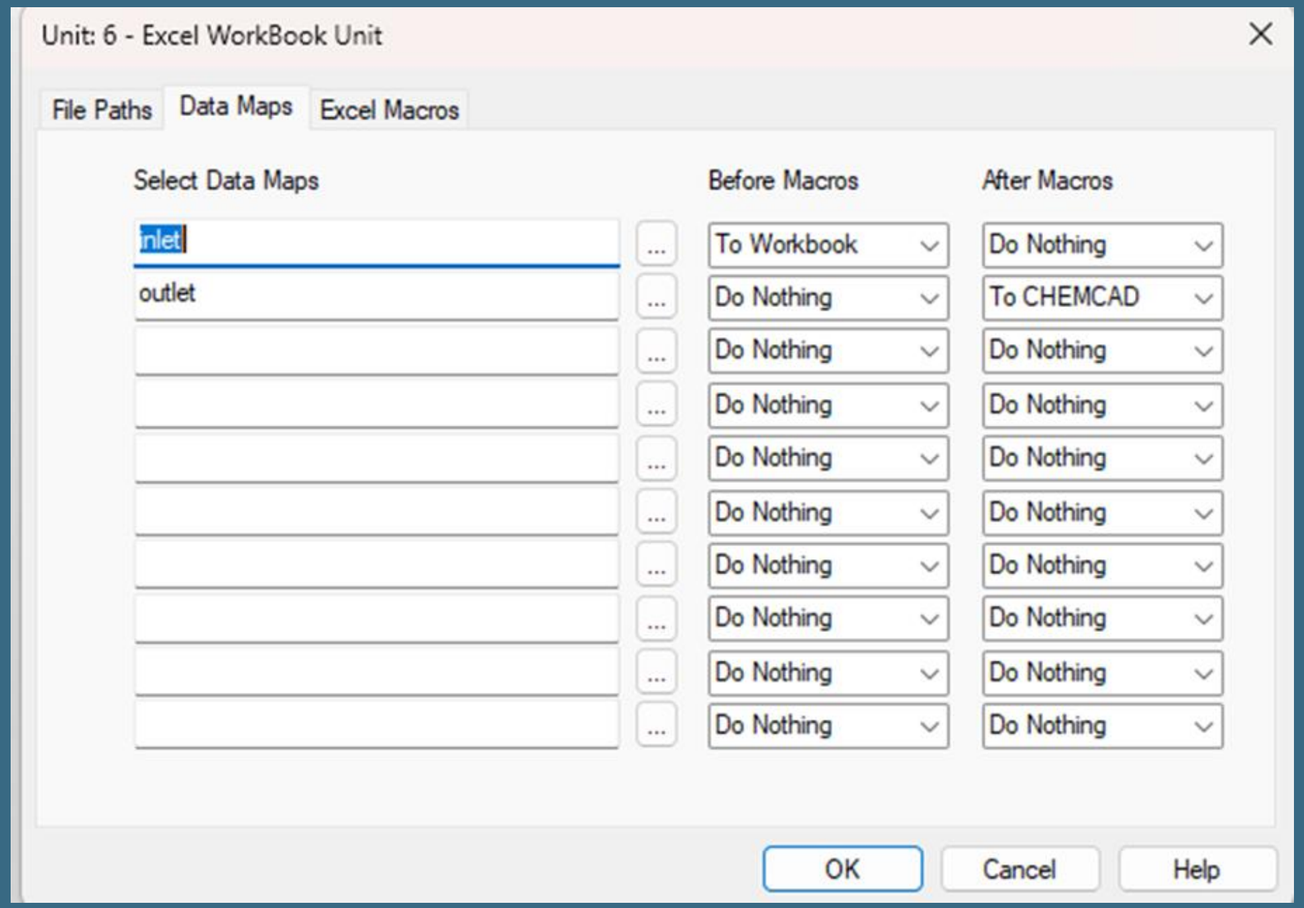

Excel Unit Operation

Data Maps

					New	Embed
	Excel Workbook Path:		MARVIN26.XLS		Browse	Open
	Excel Worksheet Name:		INSTREAMS			

Map Rule	CC Obj Type	CC Obj ID	Par ID	Component	WrkSht Cell/...	Weight
To Worksh...	Stream	2	1 Temperature	<None>	C10	1.00000
To Worksheet ...	Stream	2	2 Pressure	<None>	C11	1.00000
To Worksheet ...	Stream	2	3 Mole vap f...	<None>	C12	1.00000
To Worksheet ...	Stream	2	4 Enthalpy	<None>	C13	1.00000
To Worksheet ...	Stream	2	Comp mol...	Water	C14	1.00000
To Worksheet ...	Stream	2	Comp mol...	Oxygen	C15	1.00000
To Worksheet ...	Stream	2	Comp mol...	Nitrogen	C16	1.00000
To Worksheet ...	Stream	2	Comp mol...	Wood	C17	1.00000
To Worksheet ...	Stream	2	Comp mol...	Dibutyl Ketone	C18	1.00000
To Worksheet ...	Stream	2	Comp mol...	1-Nonanal	C19	1.00000
To Worksheet ...	Stream	2	Comp mol...	N-Decane	C20	1.00000
To Worksheet ...	Stream	2	Comp mol...	3,3,5-TriMth-C7	C21	1.00000
To Worksheet ...	Stream	2	Comp mol...	N-Nonane	C22	1.00000
To Worksheet ...	Stream	2	Comp mol...	N-Tridecane	C23	1.00000

					New	Embed
	Excel Workbook Path:		MARVIN26.XLS		Browse	Open
	Excel Worksheet Name:		OUTSTREAMS			

Map Rule	CC Obj Type	CC Obj ID	Par ID	Component	WrkSht Cell/...	Weight
To CC Only	Stream	9	1 Temperature	<None>	C10	1.00000
To CC Only	Stream	9	2 Pressure	<None>	C11	1.00000
To CC Only	Stream	9	3 Mole vap f...	<None>	C12	1.00000
To CC Only	Stream	9	4 Enthalpy	<None>	C13	1.00000
To CC Only	Stream	9	Comp mol...	Water	C14	1.00000
To CC Only	Stream	9	Comp mol...	Oxygen	C15	1.00000
To CC Only	Stream	9	Comp mol...	Nitrogen	C16	1.00000
To CC Only	Stream	9	Comp mol...	Wood	C17	1.00000
To CC Only	Stream	9	Comp mol...	Dibutyl Ketone	C18	1.00000
To CC Only	Stream	9	Comp mol...	1-Nonanal	C19	1.00000
To CC Only	Stream	9	Comp mol...	N-Decane	C20	1.00000
To CC Only	Stream	9	Comp mol...	3,3,5-TriMth-C7	C21	1.00000
To CC Only	Stream	9	Comp mol...	N-Nonane	C22	1.00000
To CC Only	Stream	9	Comp mol...	N-Tridecane	C23	1.00000

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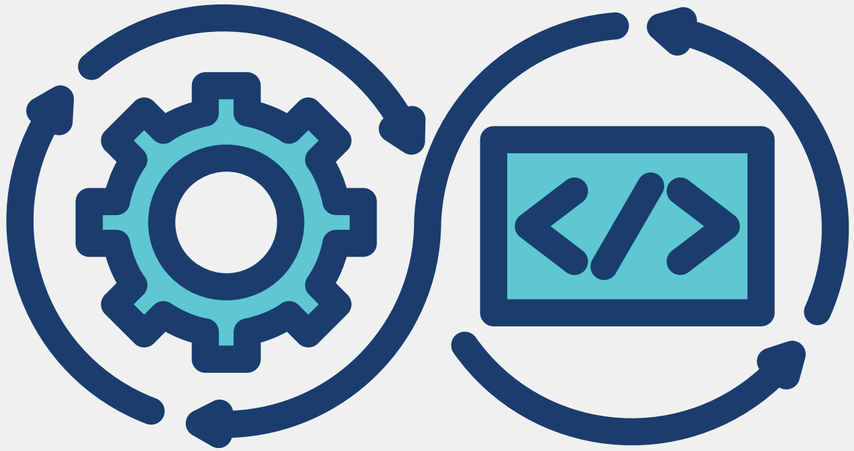
Spreadsheet

- The spreadsheet contains 4 worksheets.
- The Instreams and Outstreams sheets are tied to the Datamaps.
- The Simdata and Chart sheets are the internal calculators.

Excel Unit Operation

- The excel unit operation uses the data maps referenced.
- The input to the spreadsheet INSTREAMS is stream 2.
- The output from the spreadsheet OUTSTREAMS is stream 9.
- In this case, the temperature, pressure and composition of streams 2 and 9 are identical.
- In the spreadsheet, the composition of stream 2 is passed to the internal calculation SIMDATA, which integrates with the flammability diagram



As the simulation is run in dynamic mode, we can see the operating point of the autoclave move through the flammable envelope, starting below the LFL and moving to above the UFL.

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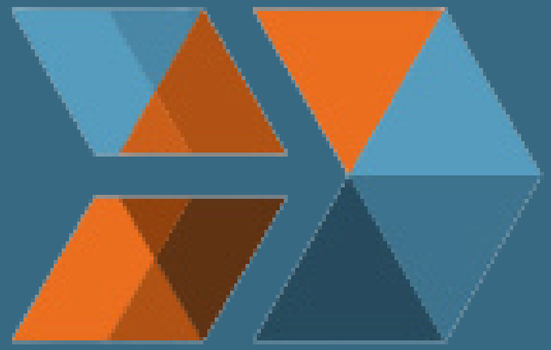
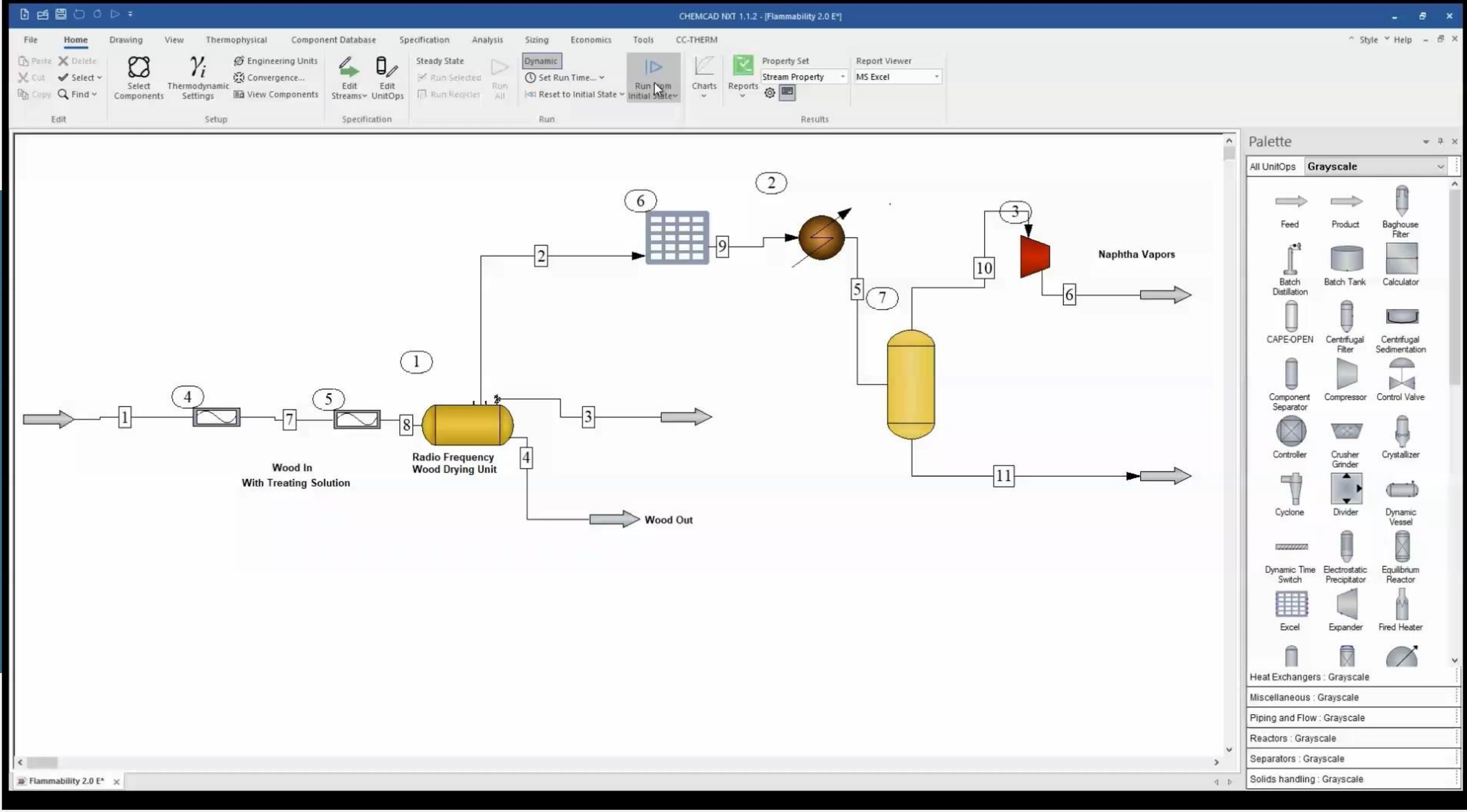
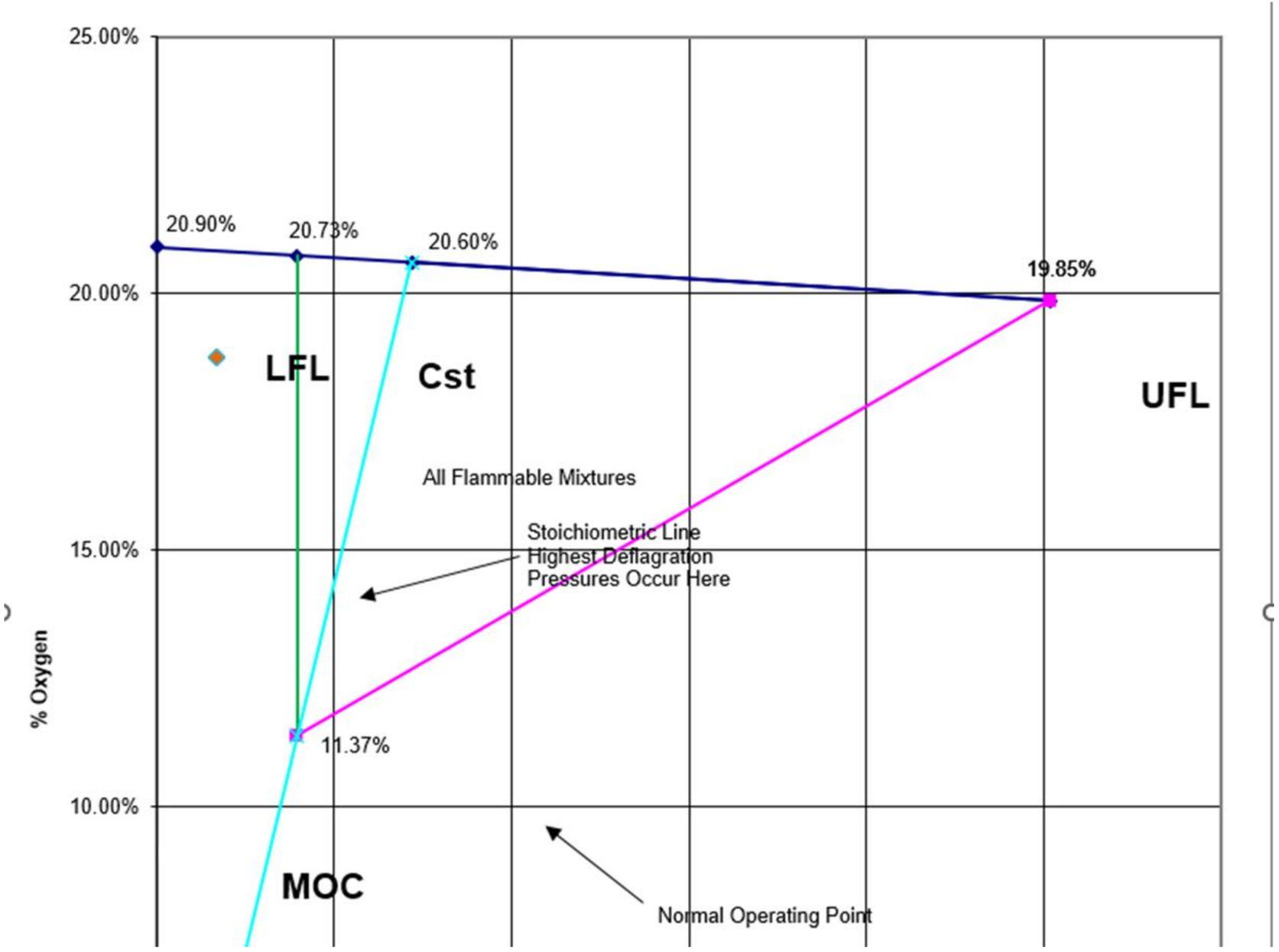
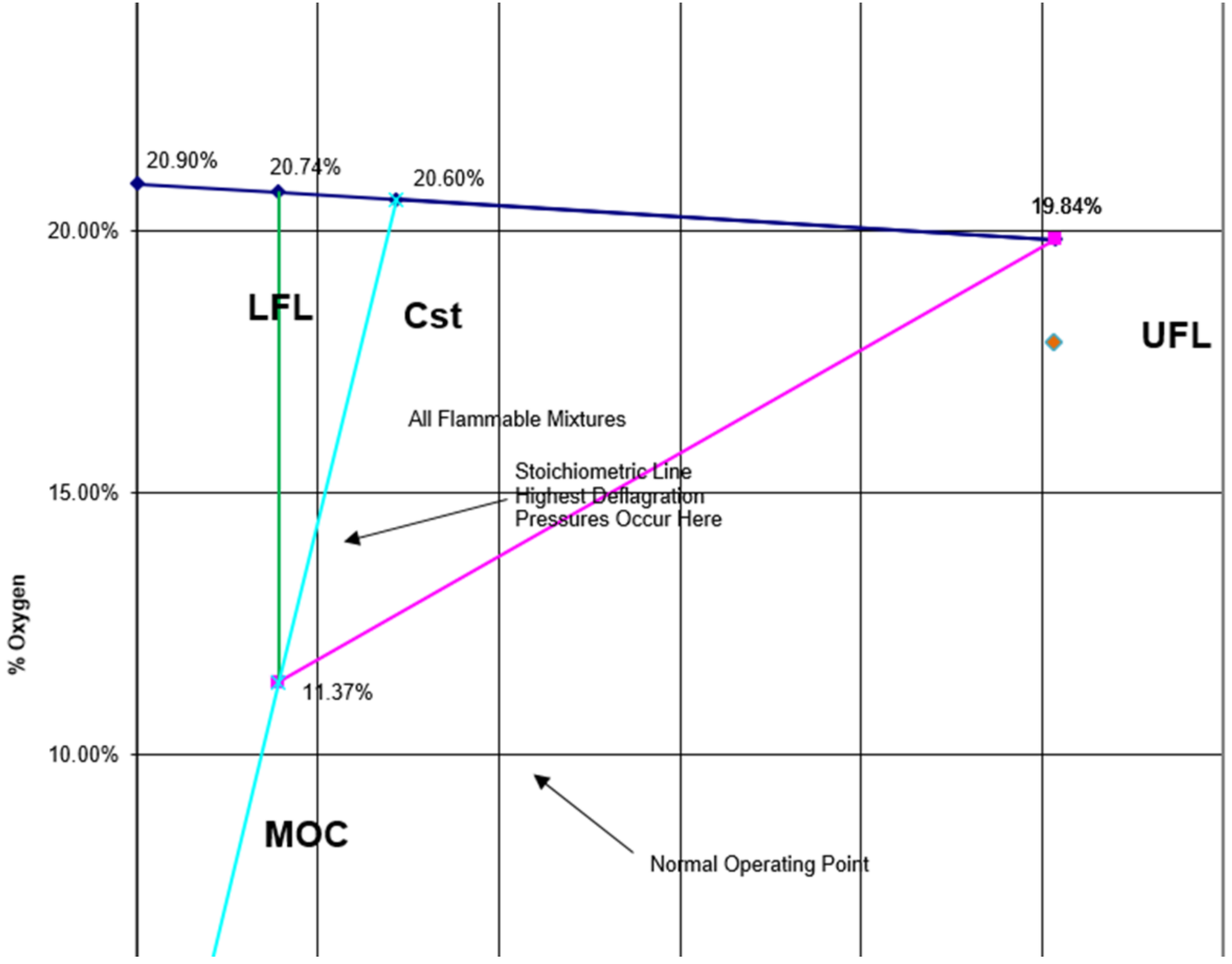
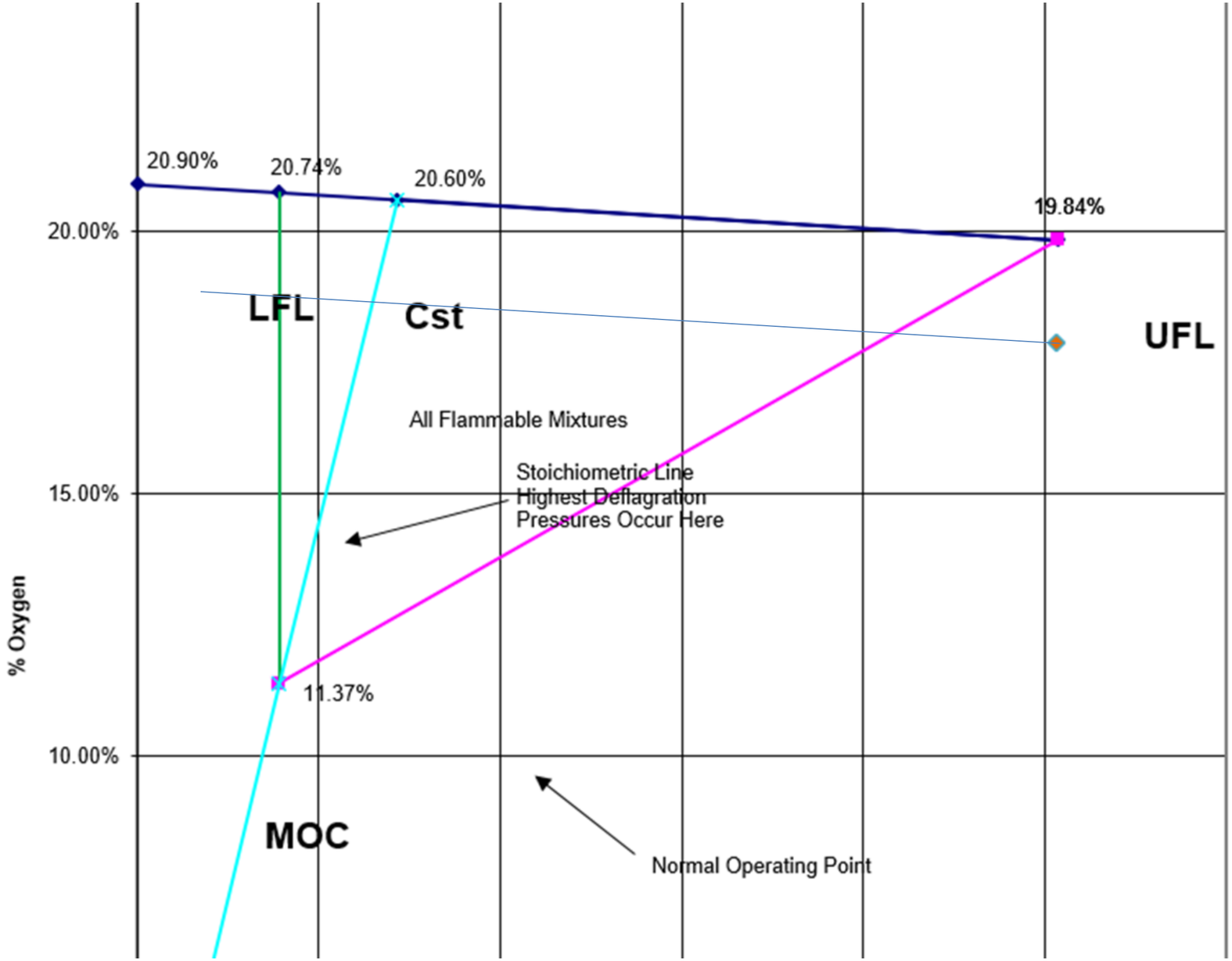
Let’s start the SIMULATION




CHEMCAD NXT 1.1.2 - [Flammability 2.0 E*]
File
Home
Drawing
View
Thermophysical
Component Database
Specification
Analysis
Sizing
Economics
Tools
CC-THERM
Style
Help
Paste
Delete
Cut
Select
Copy
Find
Edit
Select Components
Thermodynamic Settings
Engineering Units
Convergence...
View Components
Setup
Edit Streams
Edit UnitOps
Specification
Steady State
Run Selected
Run Recycle
Run All
Dynamic
Set Run Time...
Reset to Initial State
Run from Initial State
Run
Charts
Reports
Property Set
Stream Property
Report Viewer
MS Excel
Results
Naphtha Vapors
Wood In
With Treating Solution
Radio Frequency
Wood Drying Unit
Wood Out
Palette
All UnitOps
Grayscale
Feed
Product
Baghouse Filter
Batch Distillation
Batch Tank
Calculator
CAPE-OPEN
Centrifugal Filter
Centrifugal Sedimentation
Component Separator
Compressor
Control Valve
Controller
Crusher Grinder
Crystallizer
Cyclone
Divider
Dynamic Vessel
Dynamic Time Switch
Electrostatic Precipitator
Equilibrium Reactor
Excel
Expander
Fired Heater
Heat Exchangers : Grayscale
Miscellaneous : Grayscale
Piping and Flow : Grayscale
Reactors : Grayscale
Separators : Grayscale
Solids handling : Grayscale
Flammability 2.0 E*


25.00%
20.00%
15.00%
10.00%
% Oxygen
20.90%
20.73%
20.60%
19.85%
LFL
Cst
UFL
All Flammable Mixtures
Stoichiometric Line
Highest Deflagration
Pressures Occur Here
11.37%
MOC
Normal Operating Point


20.90%
20.74%
20.60%
19.84%
20.00%
LFL
Cst
UFL
All Flammable Mixtures
Stoichiometric Line
Highest Deflagration
Pressures Occur Here
15.00%
% Oxygen
11.37%
10.00%
MOC
Normal Operating Point


20.90%
20.74%
20.60%
19.84%
20.00%
LFL
Cst
UFL
All Flammable Mixtures
Stoichiometric Line
Highest Deflagration
Pressures Occur Here
15.00%
% Oxygen
11.37%
10.00%
MOC
Normal Operating Point

Conclusion

- The gas stream Number 2 was in the flammable envelope for approximately 6 minutes.
- If we move past the condenser, it is probably less flammable there since some of the hydrocarbon has condensed
- In a HAZOP and the coolant fails to the condenser then this is condition we are looking at. Stream 5 equals stream 2.
- A flashback could occur if the exhaust of the vacuum pump is connected to a thermal oxidizer.
- A deflagration arrestor is recommended with a thermocouple on the front face. This would indicate that a flashback has occurred but was stopped.

GROUP POLL

After this webinar, what is your opinion about combining Excel with process simulation?

A. It looks interesting, I will give it a try.

B. I will consider it but need more help/information.

C. I already work on custom solutions like this.

C. It is not something I am interested in doing.

Additional Comments

- The Excel unit operation is a very versatile function
- Datamapping offers additional capabilities, allowing Excel to perform independent calculations and pass them back to CHEMCAD.
- The flammability diagram is an ideal application for the Excel UnitOp.
- This excel unit operation has been used by COSTELLO in the design of crystallizers, thermal oxidizers, Fisher Tropsch reactors, and hydrocrackers.

Additional Comments

Free trial license
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For All Your Attention

THANK YOU

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