

A CAPE-OPEN Unit Operation Software Component for Solving CHEMKIN Reactor Networks Inside Process Modeling Simulations



reaction
DESIGN

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Outline

- **Introduction**
- **Project Goals**
- **WorkFlow**
- **CAPE-OPEN UO architecture**
- **Summary**

Who is Reaction Design?

- Software tool provider to the automotive, energy, and electronics markets since 1997



Technology

- **CHEMKIN**

- Most widely cited and validated kinetics software available
- Focused on accurate simulations of chemistry for:
 - * Gas Turbines
 - * Automotive engines
 - * Industrial/Utility Burners
 - * Chemical Processing and Refinery
 - * Materials and Microelectronics

- **ENERGICO applies kinetics to complex flows**

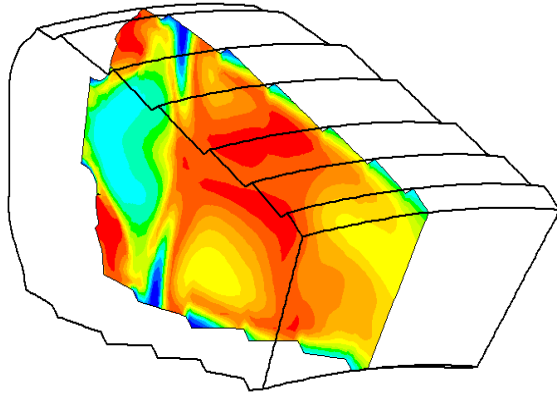
- Creates equivalent-reactor network model from CFD
- Addresses key issues for gas-turbine combustor designers
 - * Low Emissions Regulations
 - * Fuel Flexibility
 - * Combustion stability

- **Model Fuels Consortium**

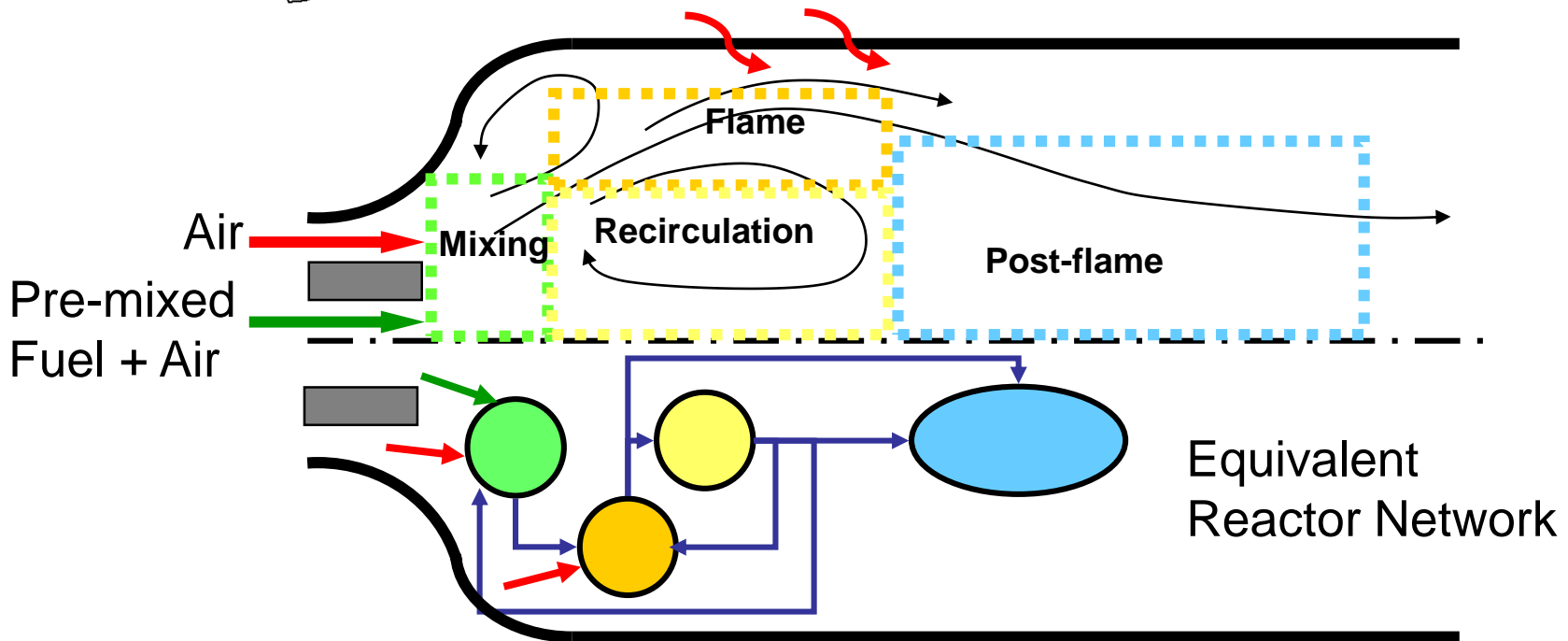
Project Goal

- NETL Project DE-FE0001074 “Package Equivalent Reactor Networks as Reduced Order Models for use with CAPE-OPEN Compliant Simulations”
- Application focus **coal-gasification plants**
- Based on ENERGICO™ and CHEMKIN-PRO® *with coal gasification extensions*
- Develop CO UO component to use ERNs in COSEs for plant design

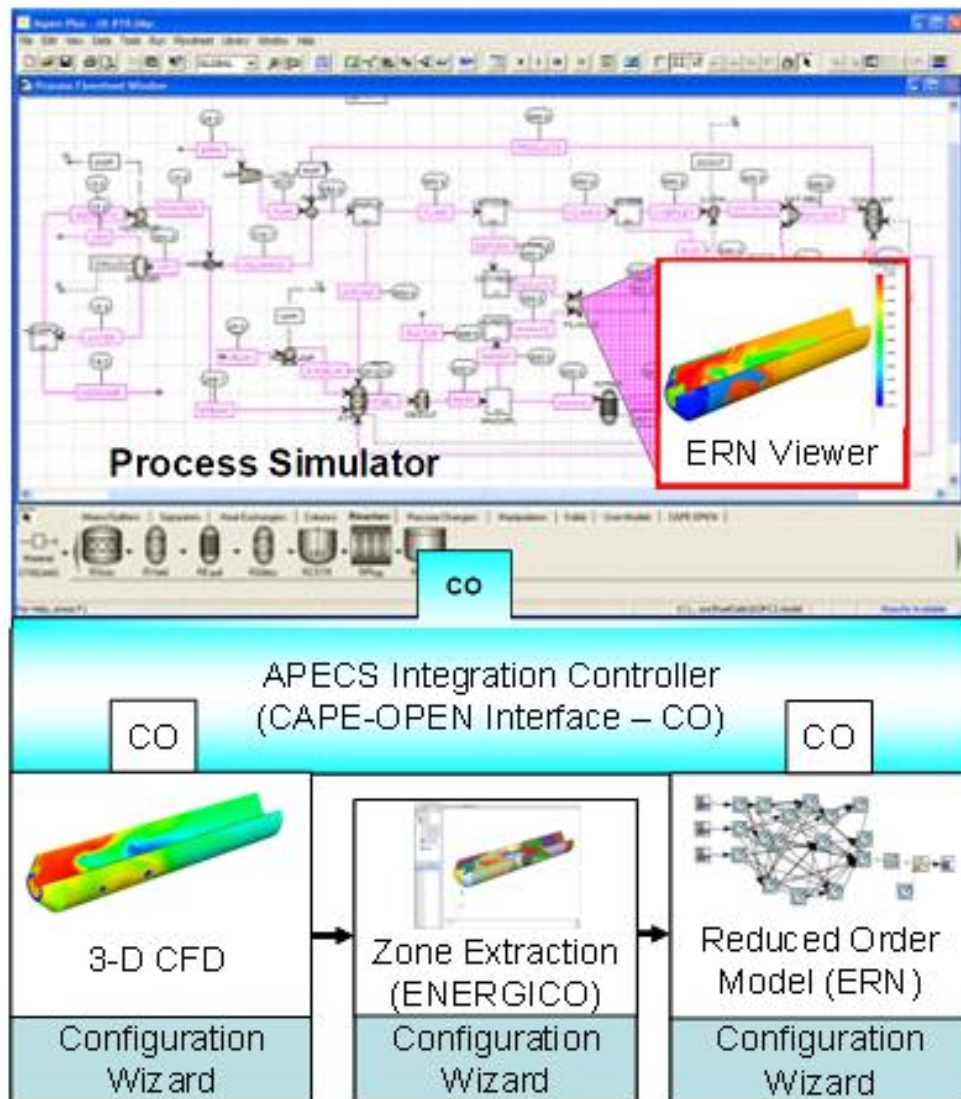
What is an ERN?



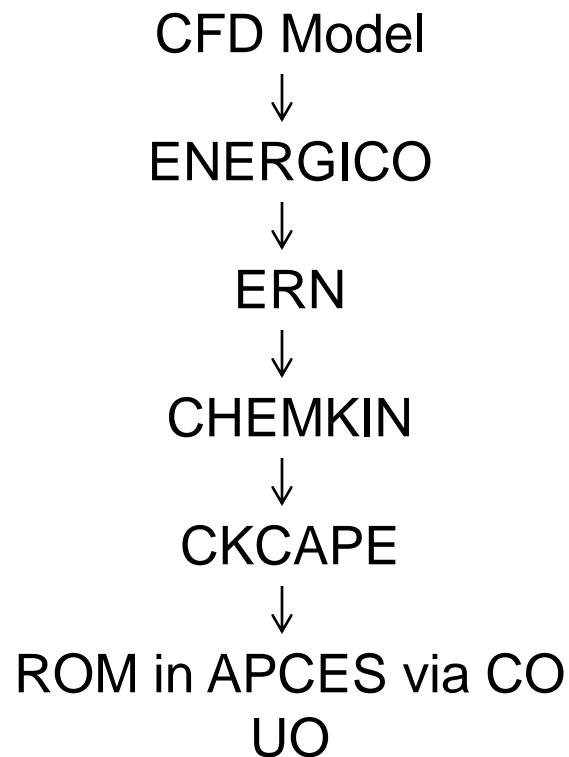
Essence of flowfield in complex geometry can be represented by reactors with mass-flow connections



NETL goal: Use ROM in APECS

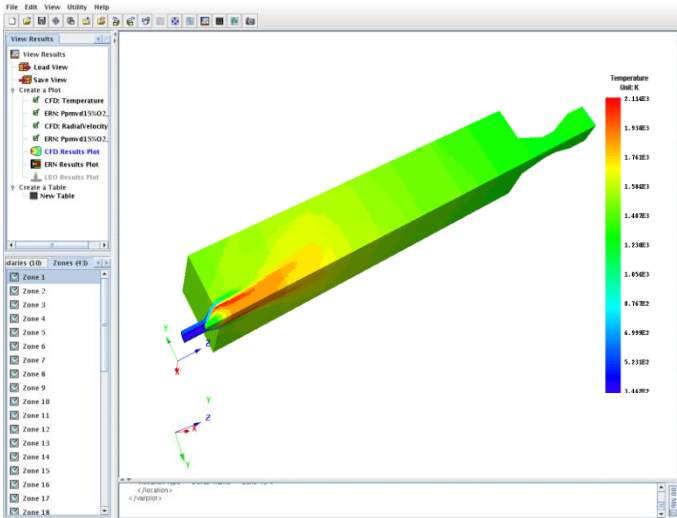


Workflow



Read CFD model into ENERIGICO

CFD Simulation results file for coal gasifier simulation



ENERIGICO User Interface

Step 1: Read CFD file into ENERIGICO



Step 2: Read in Chemistry Set

- Identify chemistry to be used in ERN

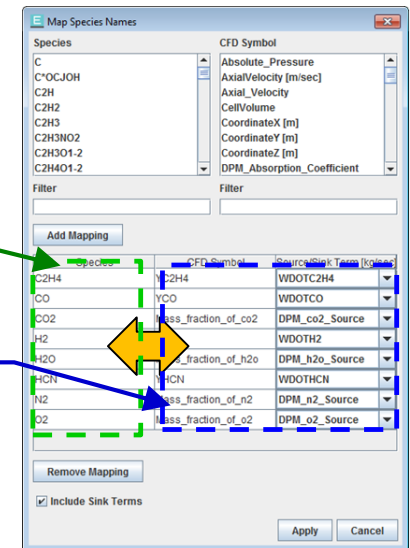


Step 3: Map Variables

- Temperature
- Pressure
- Composition

Species Symbols in
CHEMKIN mechanism

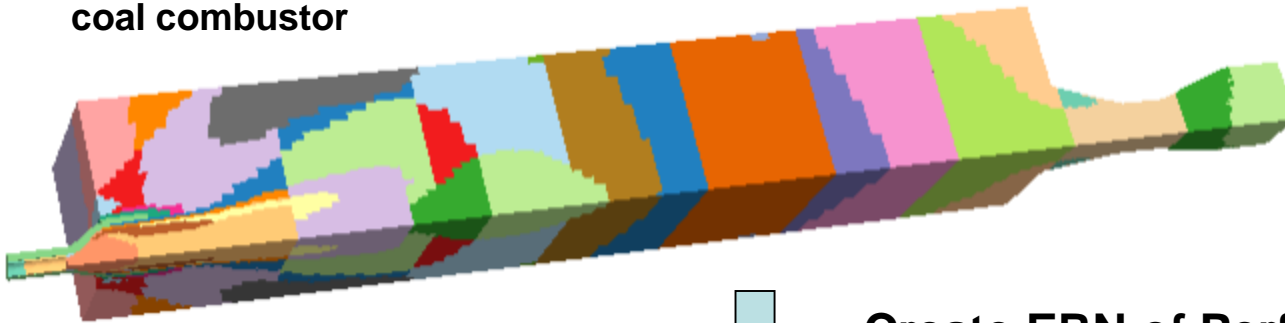
CFD variable names
and source terms



Create ERN in ENERGICO

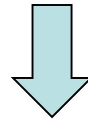
- Apply Filters to define ERN-generation algorithm within ENERGICO

47-zone partition of a coal combustor



Create Zones

- Filter: Mass_fraction_of_o2
- Filter: Mass_sources
- Filter: CoordinateZ
- Filter: VelocityZ
- Filter: CoordinateZ
- Filter: Temperature



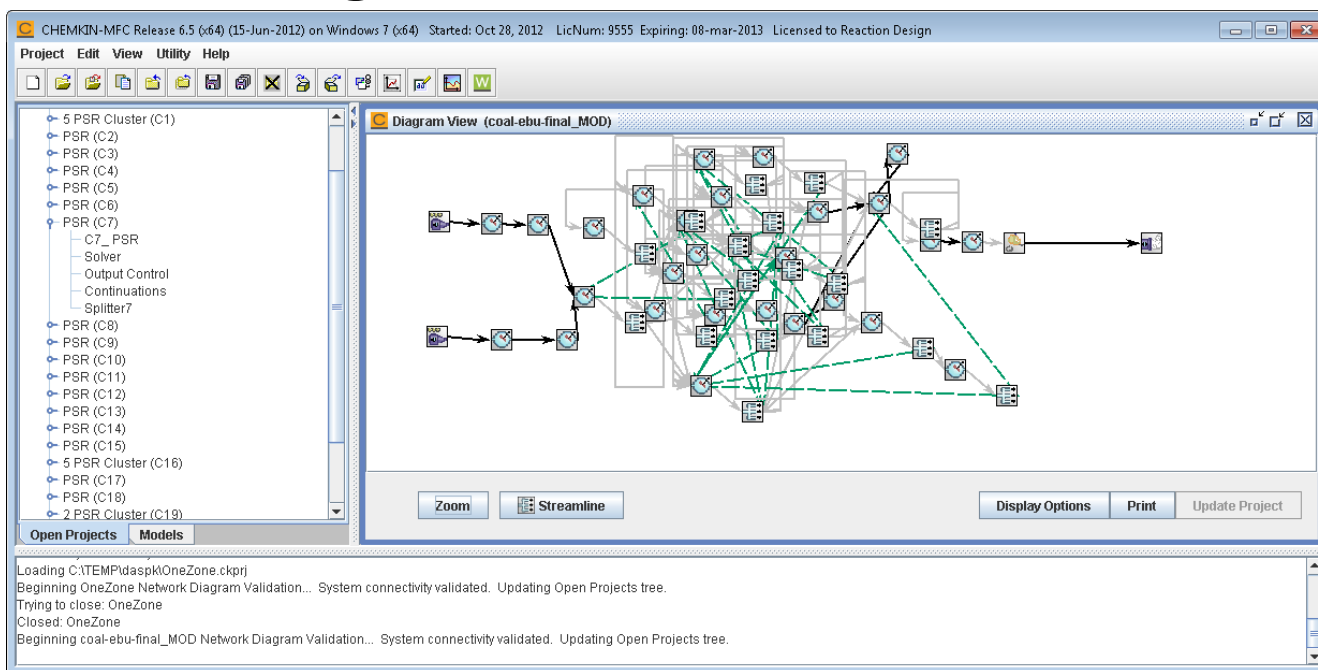
Create ERN of Perfectly Stirred Reactors, with tearing



ERN based on the 47-zone partition for the FLUENT gasifier case

Configure ERN in CHEMKIN

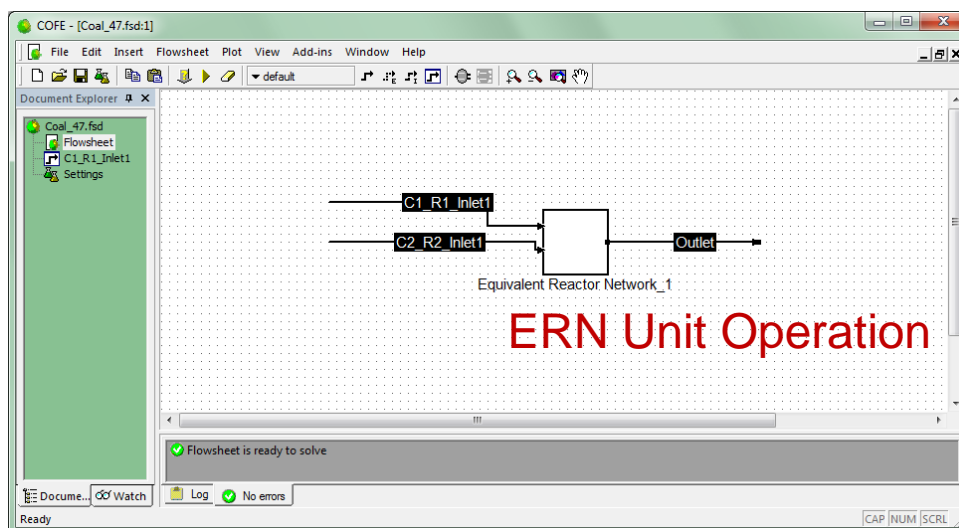
- **View and configure ERN in CHEMKIN-PRO**



- **Can solve the ERN and visualize results in ENERGICO**
- **Can tweak solver options, clustering etc**
- **Export** as CKCAPE file for CO UO DLL

CAPE OPEN Unit Operation ERN DLL

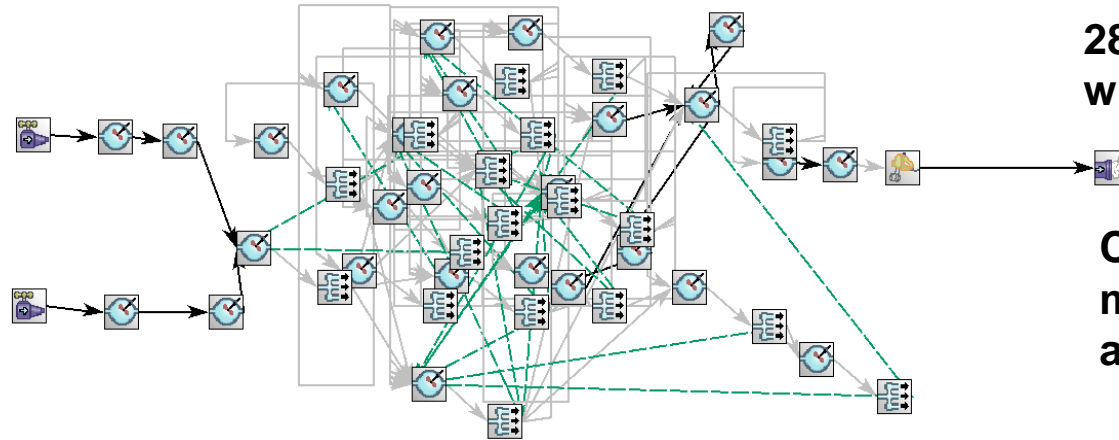
- Instance CO UO ERN in COSE from CKCAPE



- Solve as ROM in Flowsheet!
- Detailed chemistry in ERN provides additional information such as NO_x emissions

Verification

- **FLUENT 3D coal combustor tutorial**



**28-PSR network
with tearing**

**C₂-NO_x detailed chemistry
mechanism: 99 species
and 693 reactions**

Variable in Outlet Stream	CHEMKIN	COFE
Temperature (K)	1365	1365
Methane	5.489E-15	5.490E-15
Oxygen	3.554E-2	3.553E-2
Nitrogen	7.628E-1	7.638E-1
Carbon monoxide	4.558E-7	4.559E-7
Carbon dioxide	1.455E-1	1.454E-1
Hydrogen	8.072E-8	8.073E-8
Ethylene	9.519E-7	9.519E-7
Water	5.512E-1	5.512E-1
Hydrogen cyanide	9.555E-12	9.555E-12

- **89s on 4-core Intel Xeon W3564 3.20Ghz**

CO UO architecture

- **VS2005 C++ project, based on Mixer-Splitter example from Jasper M. Van Baten**
- **Loads core DLLs: chemistry pre-processor and PSR reactor model + solver**
- **Simple GUI**
- **CO UO ERN solver up to 3.6x faster than CHEMKIN**
- **BUT, what about**
 - 64bit?
 - VS2012?
 - Linux?

Summary

- **Developed ERN CO UO DLL for solving ERNs in COSEs**
- **Developed coal mechanism and models for using ERNs in NETL APECS for coal gasification**
- **Currently making CO UO ERN a supportable product**
- **Need for CO UO implementation to stay current**

Thank You