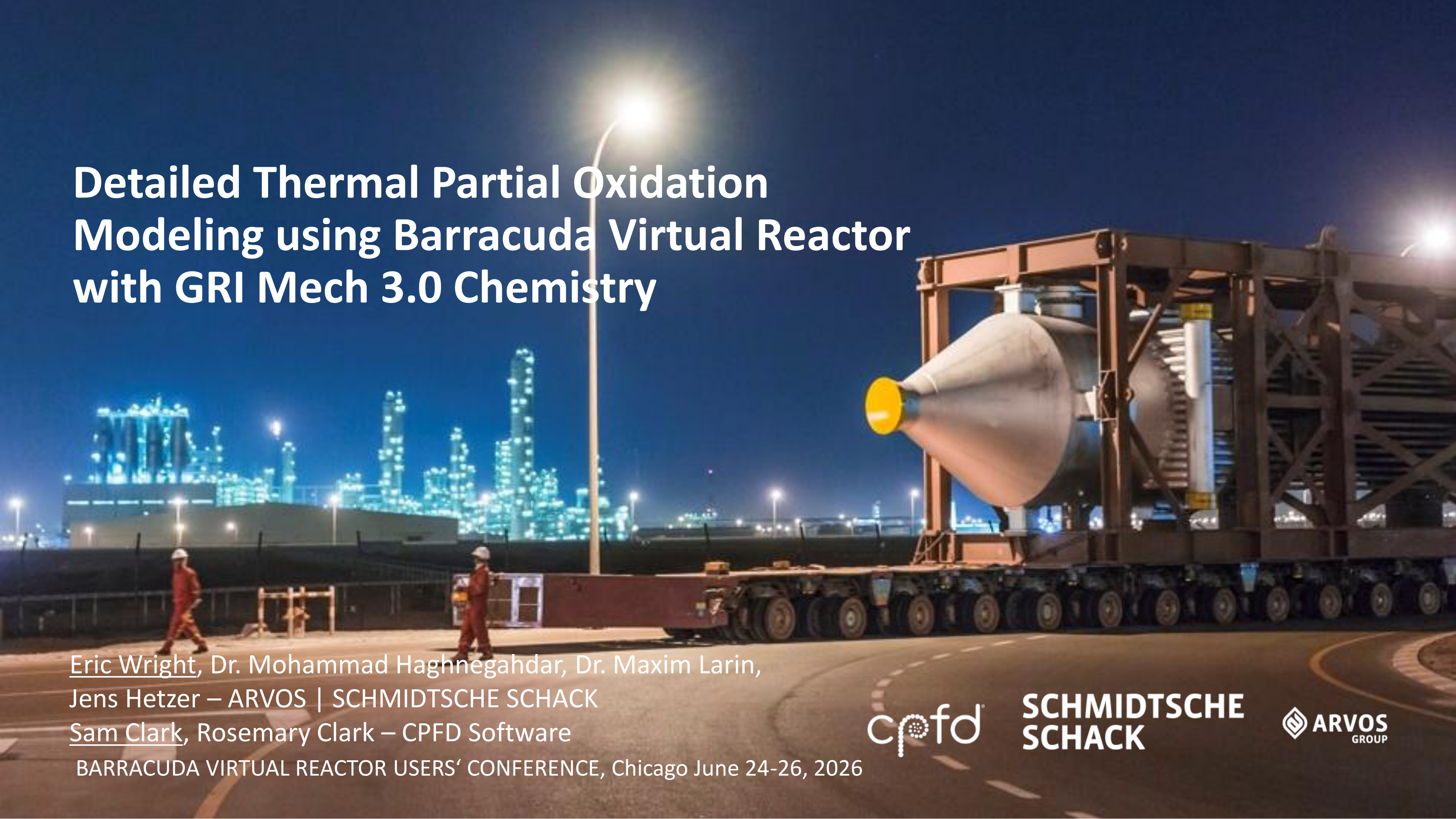


Detailed Thermal Partial Oxidation Modeling using Barracuda Virtual Reactor with GRI Mech 3.0 Chemistry

Eric Wright, Dr. Mohammad Haghnegahdar, Dr. Maxim Larin,
Jens Hetzer – ARVOS | SCHMIDTSCHE SCHACK
Sam Clark, Rosemary Clark – CPFD Software

BARRACUDA VIRTUAL REACTOR USERS‘ CONFERENCE, Chicago June 24-26, 2026

SCHMIDTSCHE SCHACK | ARVOS AT A GLANCE

EXPERIENCE IN CRITICAL HEAT TRANSFER SOLUTIONS FOR MORE THAN 110 YEARS

150+ Mio€ revenue

400+ Employees

7 Locations worldwide

2 Own manufacturing facilities

Petrochemical Industry

Waste to Value Industry

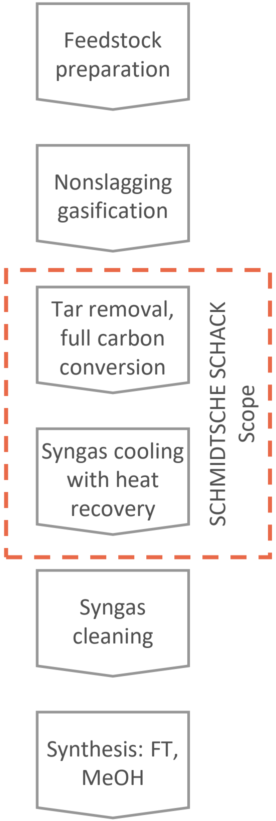
Part of your process

Refining Industry

Chemical Industry

Metallurgical Industry

GASIFICATION OF BIOMASS OR WASTE


Feedstock preparation

Nonslagging gasification

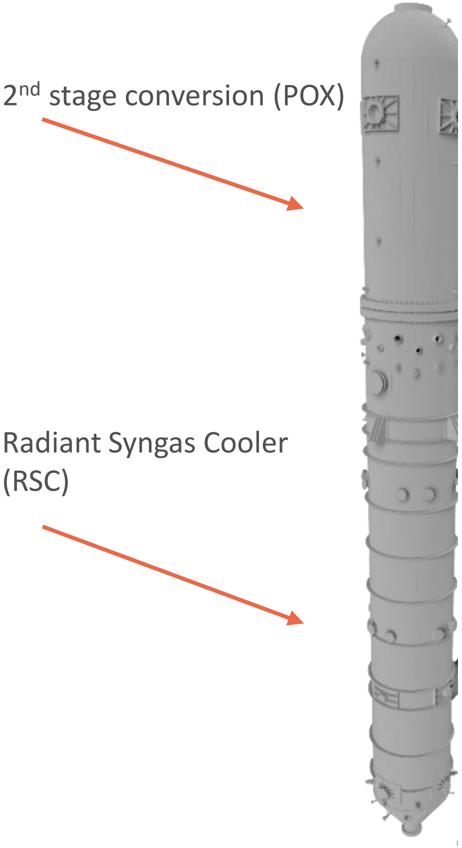
Tar removal, full carbon conversion

Syngas cooling with heat recovery

SCHMIDTSCHE SCHACK Scope

Syngas cleaning

Synthesis: FT, MeOH


2nd stage conversion (POX)

Radiant Syngas Cooler (RSC)

Application

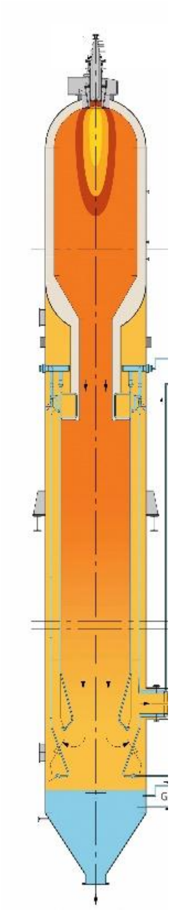
- Second conversion step by **P**artial **OX**idation to crack tars and convert Carbon from upstream Biomass or MSW gasification
- Syngas cooling with heat recovery, steam generation and super-heating
- Ash and slag handling

Simulation and Design

- POX:
  - Aspen Plus® and GRI Mech 3.0 for gas phase reactions
  - HSC Chemistry® for gas / particle reactions
- RSC: Ansys CFX for flow simulation and heat transfer

Reliable design process but no end-to-end simulation

MODEL SET-UP



POX reactor

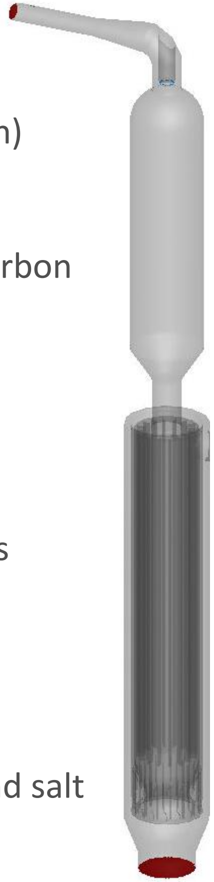
- Syngas + particles (Carbon, ash)
- Chemical reactions
  - Tar cracking
  - Reaction of unconverted Carbon and ash with syngas

Syngas Cooler

- Syngas + particles
- Chemical reactions
- Cooling of syngas and particles

Water Sump

- Evaporation by hot syngas
- Solubility of syngas traces
- Ash falling into water sump and salt formation



Model

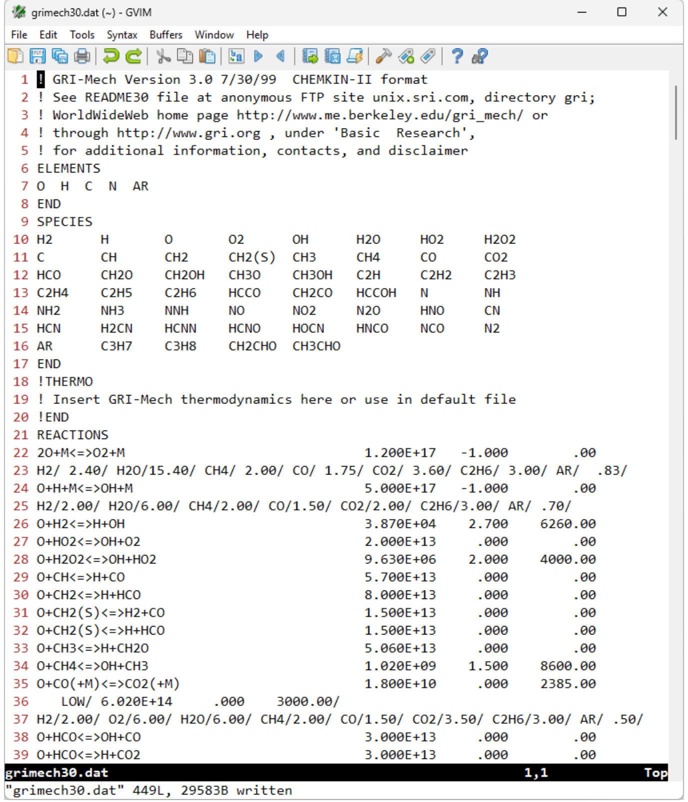
- Thermal, chemically reacting, transient, 3-dimensional
- Boundary conditions:
  - Gas and particle at inlet
  - Thermal walls for heat extraction in RSC
  - Flow condition at water sump that particles can exit

Simplifications

- No reaction of ash with particles, only Carbon particles can react
- Water sump: no evaporation, solubility, salt formation

GRI MECH 3.0 CHEMISTRY SET

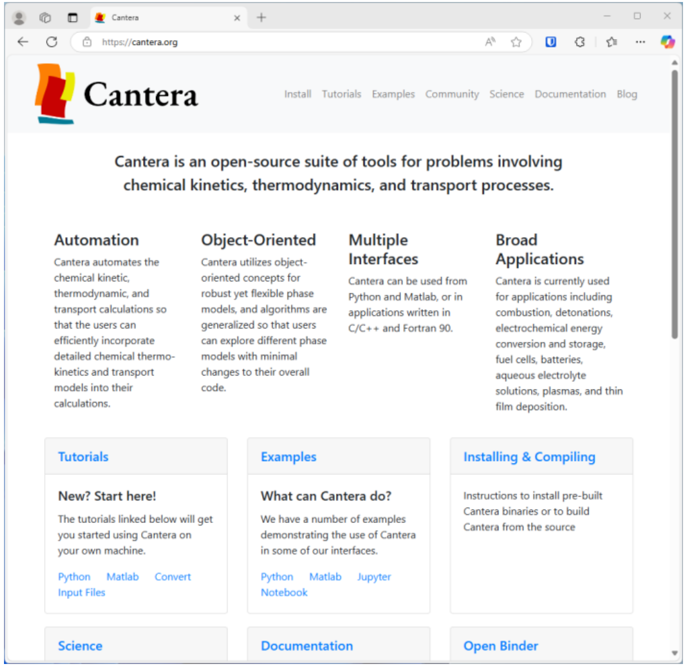
- Well-known chemistry set for modeling natural gas combustion openly available for download in Chemkin-II format
- http://www.me.berkeley.edu/gri_mech/
  - Gregory P. Smith, David M. Golden, Michael Frenklach, Nigel W. Moriarty, Boris Eiteneer, Mikhail Goldenberg, C. Thomas Bowman, Ronald K. Hanson, Soonho Song, William C. Gardiner, Jr., Vitali V. Lissianski, and Zhiwei Qin
- 325 reactions involving 53 gas species



```
! GRI-Mech Version 3.0 7/30/99  CHEMKIN-II format
! See README30 file at anonymous FTP site unix.sri.com, directory gri;
! WorldWideWeb home page http://www.me.berkeley.edu/gri_mech/ or
! through http://www.gri.org , under 'Basic  Research',
! for additional information, contacts, and disclaimer
ELEMENTS
O   H   C   N   AR
END
SPECIES
H2      H       O       O2      OH      H2O     HO2     H2O2
C       CH      CH2     CH2(S)  CH3     CH4     CO      CO2
HCO     CH2O    CH2OH   CH3O    CH3OH   C2H     C2H2    C2H3
C2H4    C2H5    C2H6    HCCO    CH2CO   HCCOH   N       NH
NH2     NH3     NNH     NO      NO2     N2O     HNO     CN
HCN     H2CN    HCNN    HCNO    HOCN    HNCO    NCO     N2
AR      C3H7    C3H8    CH2CHO  CH3CHO
END
!THERMO
! Insert GRI-Mech thermodynamics here or use in default file
!END
REACTIONS
2O+M<=>O2+M                              1.200E+17   -1.000        .00
H2/ 2.40/ H2O/15.40/ CH4/ 2.00/ CO/ 1.75/ CO2/ 3.60/ C2H6/ 3.00/ AR/  .83/
O+H+M<=>OH+M                             5.000E+17   -1.000        .00
H2/2.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/2.00/ C2H6/3.00/ AR/ .70/
O+H2<=>H+OH                              3.870E+04    2.700    6260.00
O+HO2<=>OH+O2                            2.000E+13     .000        .00
O+H2O2<=>OH+HO2                          9.630E+06    2.000    4000.00
O+CH<=>H+CO                              5.700E+13     .000        .00
O+CH2<=>H+HCO                            8.000E+13     .000        .00
O+CH2(S)<=>H2+CO                         1.500E+13     .000        .00
O+CH2(S)<=>H+HCO                         1.500E+13     .000        .00
O+CH3<=>H+CH2O                           5.060E+13     .000        .00
O+CH4<=>OH+CH3                           1.020E+09    1.500    8600.00
O+CO(+M)<=>CO2(+M)                       1.800E+10     .000    2385.00
   LOW/ 6.020E+14     .000    3000.00/
H2/2.00/ O2/6.00/ H2O/6.00/ CH4/2.00/ CO/1.50/ CO2/3.50/ C2H6/3.00/ AR/ .50/
O+HCO<=>OH+CO                            3.000E+13     .000        .00
O+HCO<=>H+CO2                            3.000E+13     .000        .00
grimech30.dat                                               1,1         Top
"grimech30.dat" 449L, 29583B written
```

USING CANTERA AS A TRANSLATION LAYER

- Cantera was used to translate the original GRI Mech 3.0 reaction set into Barracuda's project file format
- Cantera has GRI Mech 3.0 included in its distribution, which makes accessing information about species, reactions, and kinetics more convenient
- Python scripts were used to generate sections of the Barracuda Virtual Reactor project file for:
  - Base material definitions (properties for all species)
  - Reaction rate coefficients
  - Reaction definitions



Cantera is an open-source suite of tools for problems involving chemical kinetics, thermodynamics, and transport processes.

Automation

Cantera automates the chemical kinetic, thermodynamic, and transport calculations so that the users can efficiently incorporate detailed chemical thermo-kinetics and transport models into their calculations.

Object-Oriented

Cantera utilizes object-oriented concepts for robust yet flexible phase models, and algorithms are generalized so that users can explore different phase models with minimal changes to their overall code.

Multiple Interfaces

Cantera can be used from Python and Matlab, or in applications written in C/C++ and Fortran 90.

Broad Applications

Cantera is currently used for applications including combustion, detonations, electrochemical energy conversion and storage, fuel cells, batteries, aqueous electrolyte solutions, plasmas, and thin film deposition.

Tutorials

New? Start here!

The tutorials linked below will get you started using Cantera on your own machine.

Python Matlab Convert Input Files

Examples

What can Cantera do?

We have a number of examples demonstrating the use of Cantera in some of our interfaces.

Python Matlab Jupyter Notebook

Installing & Compiling

Instructions to install pre-built Cantera binaries or to build Cantera from the source

Science

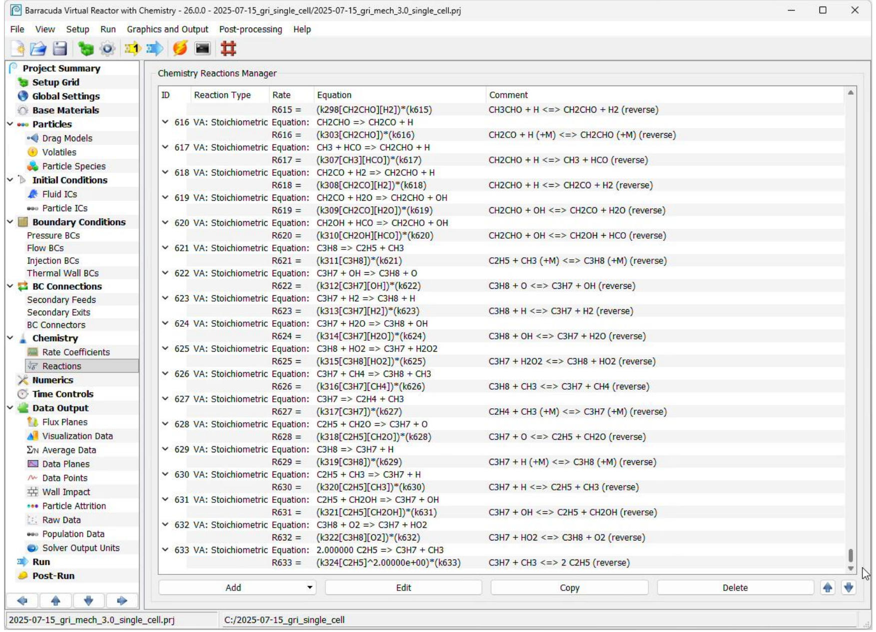
Documentation

Open Binder

https://cantera.org

GRI MECH 3.0 REACTION SET IN BARRACUDA

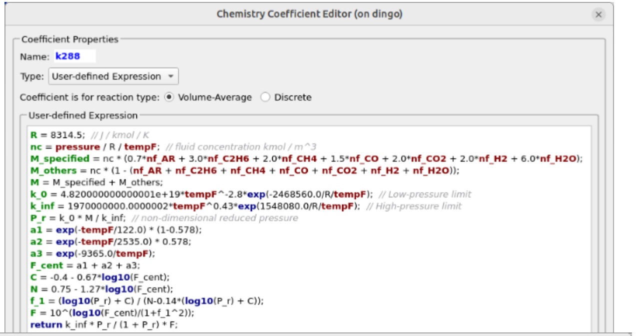
- 634 reactions total (325 forward and 309 reverse)
- Largest chemistry set known to have been implemented in a Barracuda Virtual Reactor model
- Validated by comparing single-cell Virtual Reactor simulation results with reaction rates calculated by Cantera at a known condition



ID	Reaction Type	Rate	Equation	Comment
		R615 =	(k298[CH2CHO][H2])*(k615)	CH3CHO + H <=> CH2CHO + H2 (reverse)
616	VA: Stoichiometric	Equation:	CH2CHO => CH2CO + H	
		R616 =	(k303[CH2CHO])*(k616)	CH2CO + H (+M) <=> CH2CHO (+M) (reverse)
617	VA: Stoichiometric	Equation:	CH3 + HCO => CH2CHO + H	
		R617 =	(k307[CH3][HCO])*(k617)	CH2CHO + H <=> CH3 + HCO (reverse)
618	VA: Stoichiometric	Equation:	CH2CO + H2 => CH2CHO + H	
		R618 =	(k308[CH2CO][H2])*(k618)	CH2CHO + H <=> CH2CO + H2 (reverse)
619	VA: Stoichiometric	Equation:	CH2CO + H2O => CH2CHO + OH	
		R619 =	(k309[CH2CO][H2O])*(k619)	CH2CHO + OH <=> CH2CO + H2O (reverse)
620	VA: Stoichiometric	Equation:	CH2OH + HCO => CH2CHO + OH	
		R620 =	(k310[CH2OH][HCO])*(k620)	CH2CHO + OH <=> CH2OH + HCO (reverse)
621	VA: Stoichiometric	Equation:	C3H8 => C2H5 + CH3	
		R621 =	(k311[C3H8])*(k621)	C2H5 + CH3 (+M) <=> C3H8 (+M) (reverse)
622	VA: Stoichiometric	Equation:	C3H7 + OH => C3H8 + O	
		R622 =	(k312[C3H7][OH])*(k622)	C3H8 + O <=> C3H7 + OH (reverse)
623	VA: Stoichiometric	Equation:	C3H7 + H2 => C3H8 + H	
		R623 =	(k313[C3H7][H2])*(k623)	C3H8 + H <=> C3H7 + H2 (reverse)
624	VA: Stoichiometric	Equation:	C3H7 + H2O => C3H8 + OH	
		R624 =	(k314[C3H7][H2O])*(k624)	C3H8 + OH <=> C3H7 + H2O (reverse)
625	VA: Stoichiometric	Equation:	C3H8 + HO2 => C3H7 + H2O2	
		R625 =	(k315[C3H8][HO2])*(k625)	C3H7 + H2O2 <=> C3H8 + HO2 (reverse)
626	VA: Stoichiometric	Equation:	C3H7 + CH4 => C3H8 + CH3	
		R626 =	(k316[C3H7][CH4])*(k626)	C3H8 + CH3 <=> C3H7 + CH4 (reverse)
627	VA: Stoichiometric	Equation:	C3H7 => C2H4 + CH3	
		R627 =	(k317[C3H7])*(k627)	C2H4 + CH3 (+M) <=> C3H7 (+M) (reverse)
628	VA: Stoichiometric	Equation:	C2H5 + CH2O => C3H7 + O	
		R628 =	(k318[C2H5][CH2O])*(k628)	C3H7 + O <=> C2H5 + CH2O (reverse)
629	VA: Stoichiometric	Equation:	C3H8 => C3H7 + H	
		R629 =	(k319[C3H8])*(k629)	C3H7 + H (+M) <=> C3H8 (+M) (reverse)
630	VA: Stoichiometric	Equation:	C2H5 + CH3 => C3H7 + H	
		R630 =	(k320[C2H5][CH3])*(k630)	C3H7 + H <=> C2H5 + CH3 (reverse)
631	VA: Stoichiometric	Equation:	C2H5 + CH2OH => C3H7 + OH	
		R631 =	(k321[C2H5][CH2OH])*(k631)	C3H7 + OH <=> C2H5 + CH2OH (reverse)
632	VA: Stoichiometric	Equation:	C3H8 + O2 => C3H7 + HO2	
		R632 =	(k322[C3H8][O2])*(k632)	C3H7 + HO2 <=> C3H8 + O2 (reverse)
633	VA: Stoichiometric	Equation:	2.000000 C2H5 => C3H7 + CH3	
		R633 =	(k324[C2H5]^2.00000e+00)*(k633)	C3H7 + CH3 <=> 2 C2H5 (reverse)

UDES EXTENSIVELY USED FOR RATE COEFFICIENTS

- UDEs provide flexibility when defining reaction rate coefficients in Barracuda Virtual Reactor
- GRI Mech 3.0 includes several complex types of rate coefficients:
    - Three-body Arrhenius
    - Lindemann Falloff
    - Troe Falloff
    - Reverse rates based on Gibbs free energy expressions

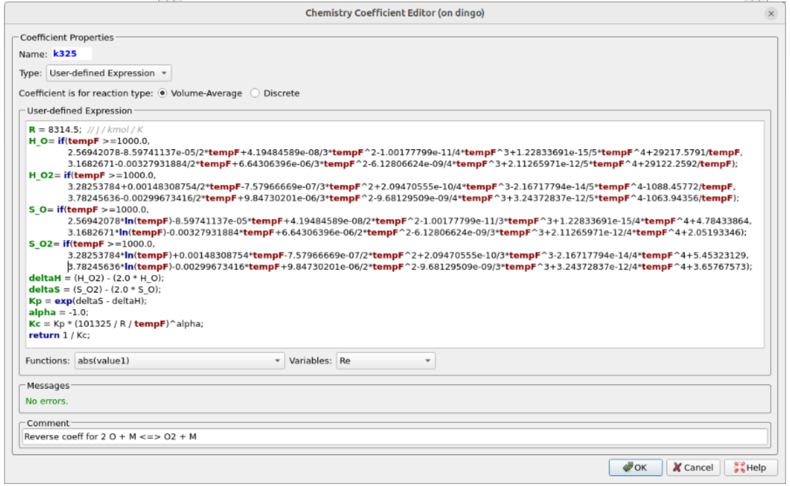


Name: k288

Type: User-defined Expression

Coefficient is for reaction type: ● Volume-Average ○ Discrete

```
R = 8314.5;  // J / kmol / K
nc = pressure / R / tempF;  // fluid concentration kmol / m^3
M_specified = nc * (0.7*nf_AR + 3.0*nf_C2H6 + 2.0*nf_CH4 + 1.5*nf_CO + 2.0*nf_CO2 + 2.0*nf_H2 + 6.0*nf_H2O);
M_others = nc * (1 - (nf_AR + nf_C2H6 + nf_CH4 + nf_CO + nf_CO2 + nf_H2 + nf_H2O));
M = M_specified + M_others;
k_0 = 4.820000000000001e+19*tempF^-2.8*exp(-2468560.0/R/tempF);  // Low-pressure limit
k_inf = 1970000000.0000002*tempF^0.43*exp(1548080.0/R/tempF);  // High-pressure limit
P_r = k_0 * M / k_inf;  // non-dimensional reduced pressure
a1 = exp(-tempF/122.0) * (1-0.578);
a2 = exp(-tempF/2535.0) * 0.578;
a3 = exp(-9365.0/tempF);
F_cent = a1 + a2 + a3;
C = -0.4 - 0.67*log10(F_cent);
N = 0.75 - 1.27*log10(F_cent);
f_1 = (log10(P_r) + C) / (N-0.14*(log10(P_r) + C));
F = 10^(log10(F_cent)/(1+f_1^2));
return k_inf * P_r / (1 + P_r) * F;
```



Name: k325

Type: User-defined Expression

Coefficient is for reaction type: ● Volume-Average ○ Discrete

```
R = 8314.5;  // J / kmol / K
H_O= if(tempF >=1000.0,
          2.56942078-8.59741137e-05/2*tempF+4.19484589e-08/3*tempF^2-1.00177799e-11/4*tempF^3+1.22833691e-15/5*tempF^4+29217.5791/tempF,
          3.1682671-0.00327931884/2*tempF+6.64306396e-06/3*tempF^2-6.12806624e-09/4*tempF^3+2.11265971e-12/5*tempF^4+29122.2592/tempF);
H_O2= if(tempF >=1000.0,
          3.28253784+0.00148308754/2*tempF-7.57966669e-07/3*tempF^2+2.09470555e-10/4*tempF^3-2.16717794e-14/5*tempF^4-1088.45772/tempF,
          3.78245636-0.00299673416/2*tempF+9.84730201e-06/3*tempF^2-9.68129509e-09/4*tempF^3+3.24372837e-12/5*tempF^4-1063.94356/tempF);
S_O= if(tempF >=1000.0,
          2.56942078*ln(tempF)-8.59741137e-05*tempF+4.19484589e-08/2*tempF^2-1.00177799e-11/3*tempF^3+1.22833691e-15/4*tempF^4+4.78433864,
          3.1682671*ln(tempF)-0.00327931884*tempF+6.64306396e-06/2*tempF^2-6.12806624e-09/3*tempF^3+2.11265971e-12/4*tempF^4+2.05193346);
S_O2= if(tempF >=1000.0,
          3.28253784*ln(tempF)+0.00148308754*tempF-7.57966669e-07/2*tempF^2+2.09470555e-10/3*tempF^3-2.16717794e-14/4*tempF^4+5.45323129,
          3.78245636*ln(tempF)-0.00299673416*tempF+9.84730201e-06/2*tempF^2-9.68129509e-09/3*tempF^3+3.24372837e-12/4*tempF^4+3.65767573);
deltaH = (H_O2) - (2.0 * H_O);
deltaS = (S_O2) - (2.0 * S_O);
Kp = exp(deltaS - deltaH);
alpha = -1.0;
Kc = Kp * (101325 / R / tempF)^alpha;
return 1 / Kc;
```

Functions: abs(value1) Variables: Re

No errors.

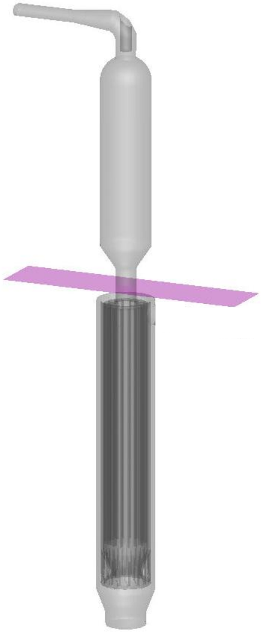
Reverse coeff for 2 O + M <=> O2 + M

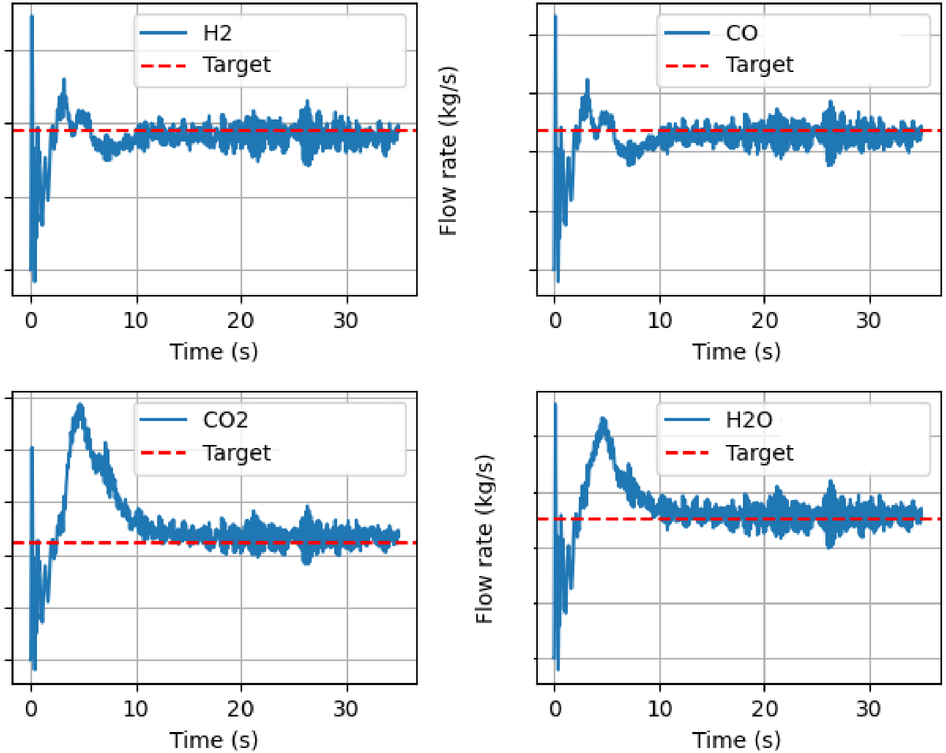
SIMULATION SPEED

- Average simulation speed: 3.5 seconds per day
- Number of real cells: 780,000
- Number of clouds: 5 million
- Total simulation time to reach t = 60 s: 16 days
- Computer hardware used:
- AMD EPYC 9174F CPU with 16 cores at 4.1 GHz (up to 4.4 GHz boost)
- 2 x NVIDIA RTX 6000 Ada GPU cards

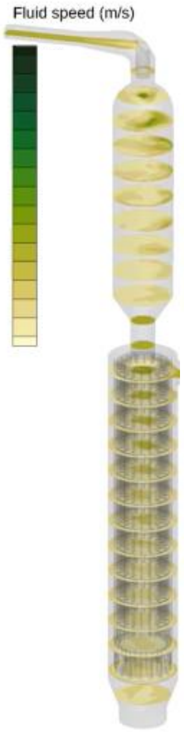
GAS SPECIES FLOW RATES AT POX EXIT

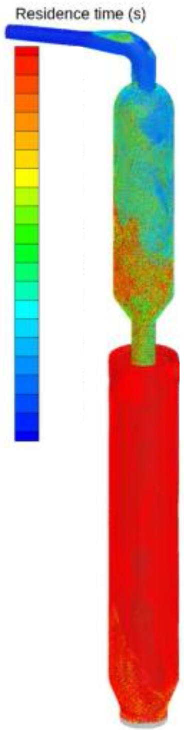
- Flux plane records mass flow rate of each gas species
- Barracuda simulation confirms Aspen Plus® simulation using GRI Mech 3.0 database, which was validated against experimental data.

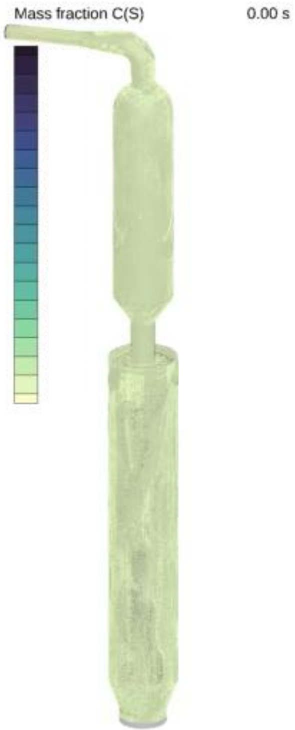




3D VIEWS OF FLUID AND PARTICLE BEHAVIOR

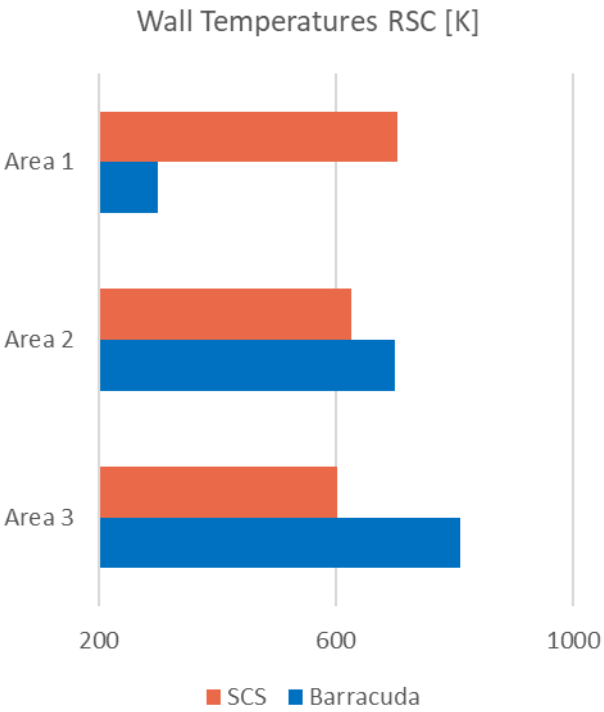


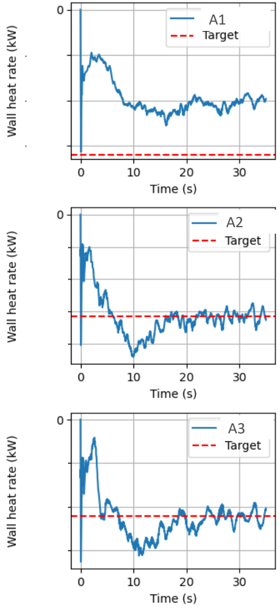




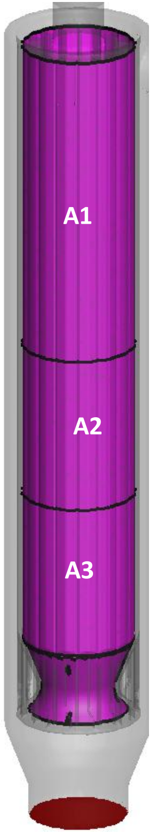
HEAT TRANSFER IN RADIANT SYNGAS COOLER

- 1st approach: specify heat flux as boundary condition in RSC
    - Target heat flux met after 20sec for area 2 and 3, but not for area 1
    - Calculated wall temperatures of RSC do not match with SCS own simulations
- 2nd approach: specify wall temperatures as BC in RSC
    - Calculated heat flux deviates ± 50% from SCS design tools, which are validated over several decades.


Wall Temperatures RSC [K]

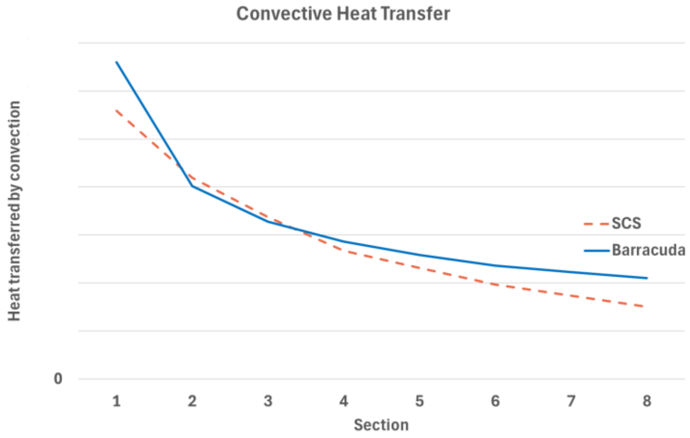


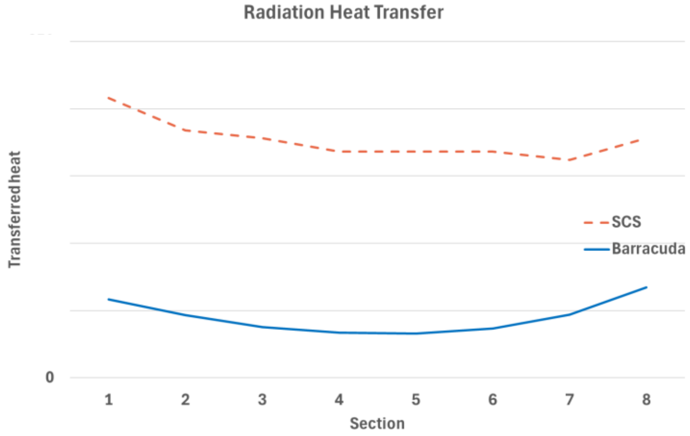
Simulation results of 1st approach



DETAILED ANALYSIS OF HEAT TRANSFER

- Reference case is a similar RSC geometry, which was simulated using Ansys CFX. Simulation results match well with SCS tools.
- Convective heat transfer: trend of Barracuda's results match with SCS reference case, but in total more heat is transferred by convection
- Radiative heat transfer: after adjusting gas absorption coefficients in Barracuda material database, trend is comparable with SCS reference, but total radiative heat transfer is underpredicted.
- Further detailed analysis required





CONCLUSIONS

- First implementation of GRI Mech 3.0 within Barracuda
- Successful modeling with 634 reactions
- Gas phase reactions results at POX reactor outlet were consistent with other models previously developed and validated by ARVOS
- Reaction rate and conversion of carbon particles confirm previous ARVOS assumptions
- Simulation provides a better understanding of the fluid-particle flow and particle separation
- Further analysis required to improve heat transfer

Thank you for your kind attention!

Eric Wright – Business Development Manager GFC America

eric.wright@arvos-group.com

www.schmidtsche-schack.com

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