Simulation of Coal Particles in a Full Chemical Looping Combustion System

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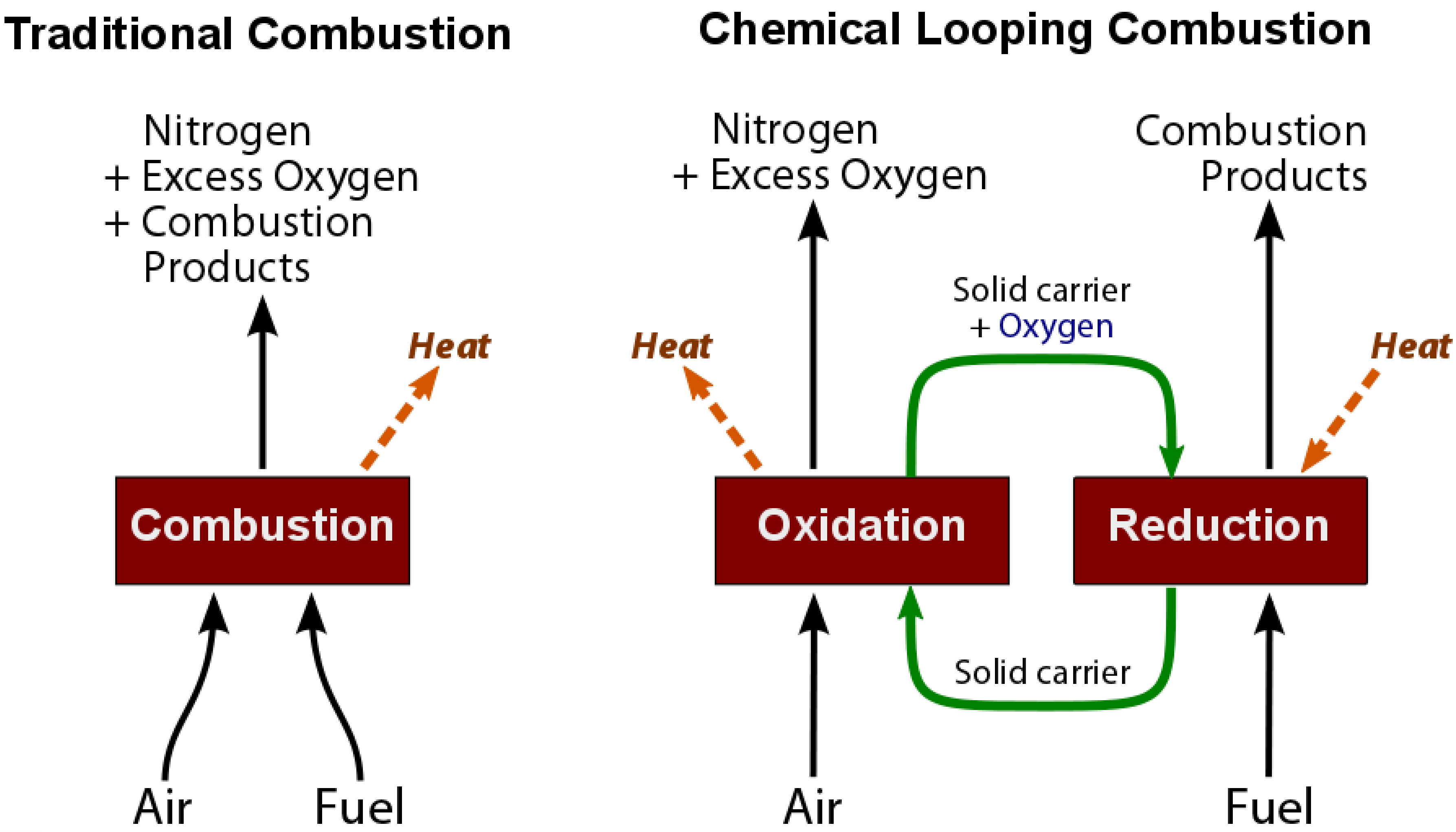
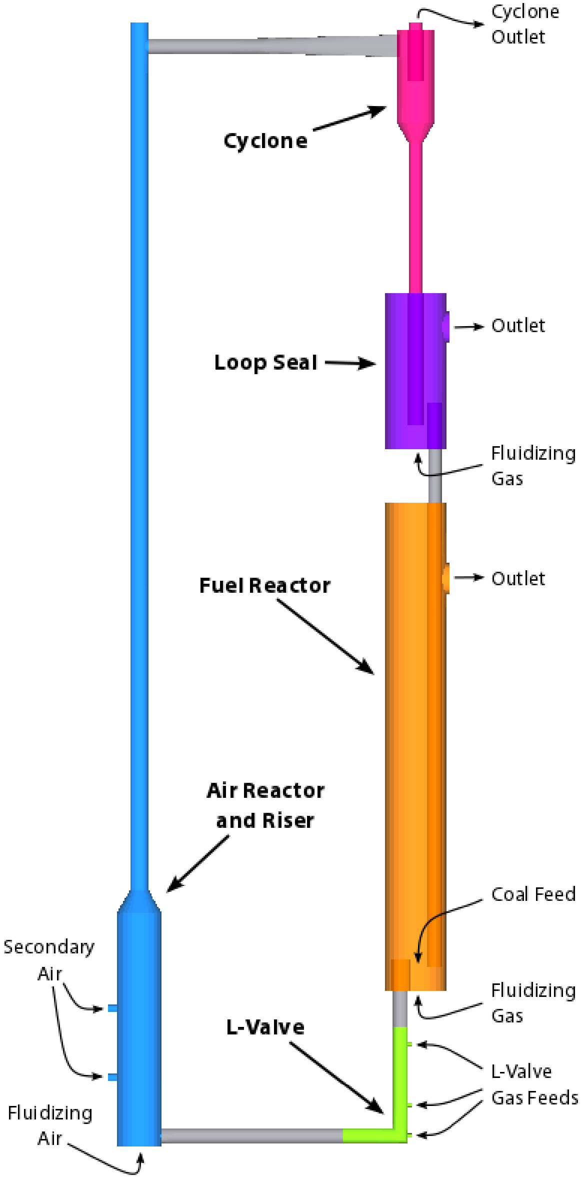
Objectives

- Develop a Chemical Looping Combustion model
  - Full loop, 3D geometry
  - Fluid-particle dynamics
  - Oxidation/reduction chemistry
  - Coal devolatilization, moisture release, gasification reactions
  - Thermal characteristics


Traditional Combustion
Nitrogen
+ Excess Oxygen
+ Combustion
Products
Heat
Combustion
Air
Fuel
Chemical Looping Combustion
Nitrogen
+ Excess Oxygen
Combustion
Products
Solid carrier
+ Oxygen
Heat
Heat
Oxidation
Reduction
Solid carrier
Air
Fuel

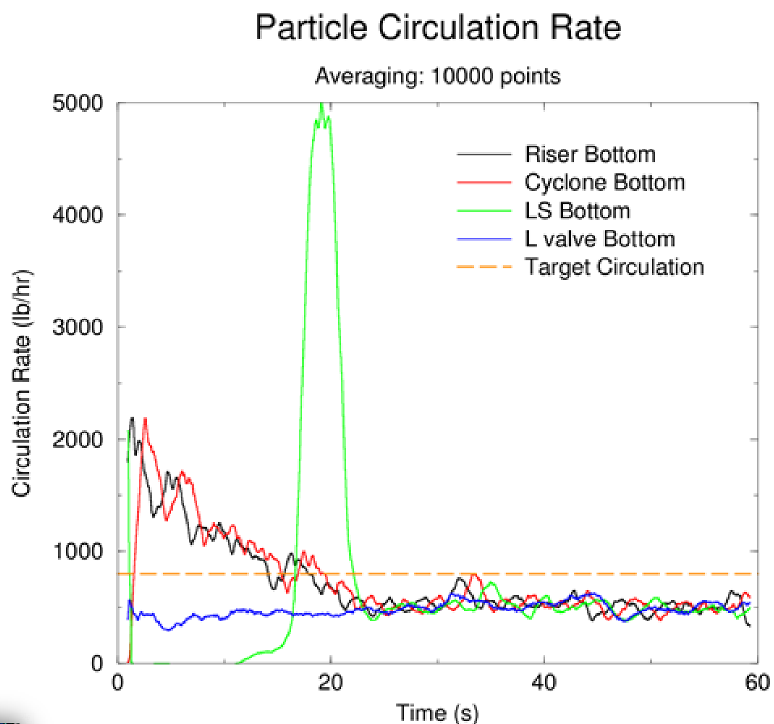
Model geometry

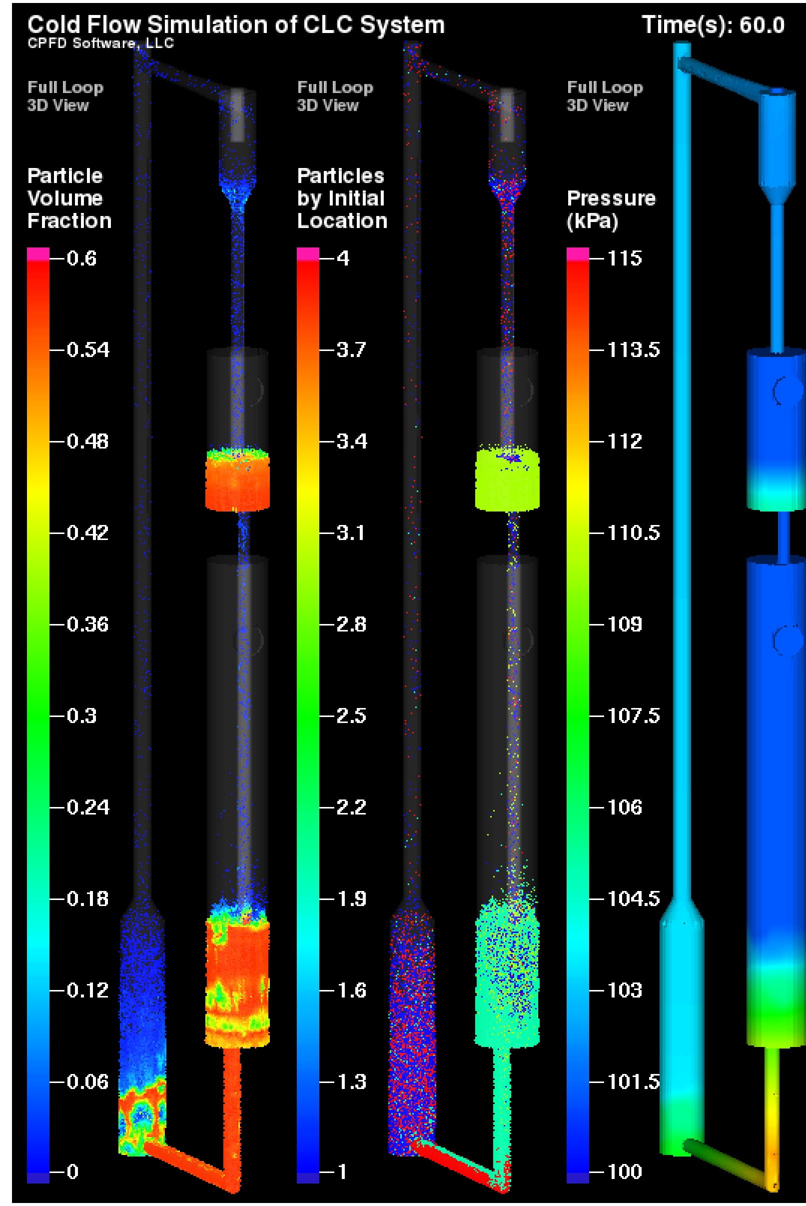
- Design provided by NETL for **800 lb/hr** circulation of solids carrier
- Approximately 12' tall
- Geometry contains equipment for reactions
  - Air reactor
  - Fuel reactor
- Solids circulation and separation
  - Cyclone
  - Loop seal
  - L-valve



Cold flow model

- Isothermal at 298K
- Non-reacting





Modeling CLC Reactions

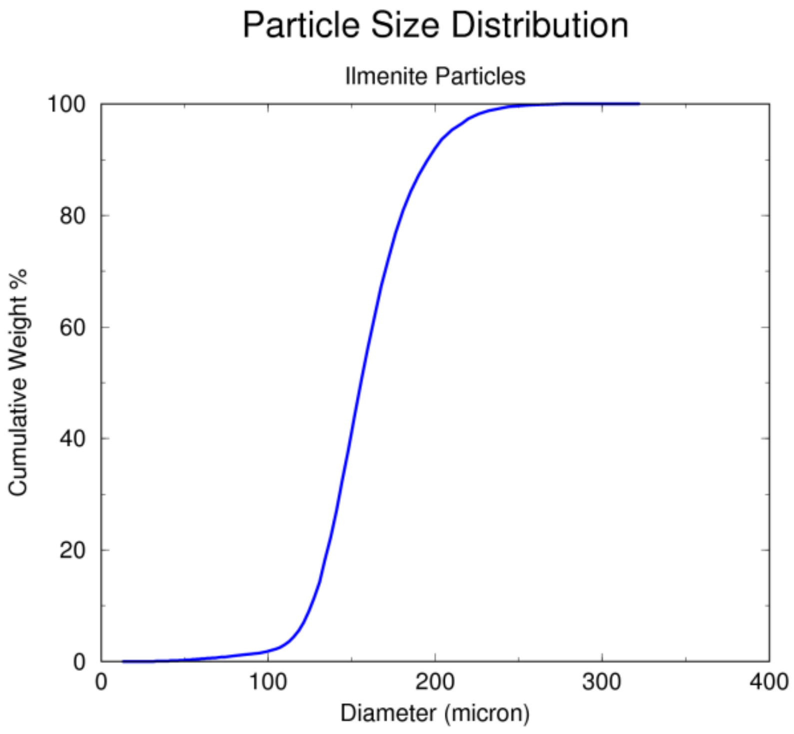
- Key features
  - Multicomponent particles
  - Particle level chemistry

- Multicomponent particles provide Lagrangian tracking of particle composition

- Particle level chemistry provides a separate domain to each computational particle for reaction calculations
  - Particle composition
  - Particle temperature
  - Particle diameter, area, etc
  - Fluid properties

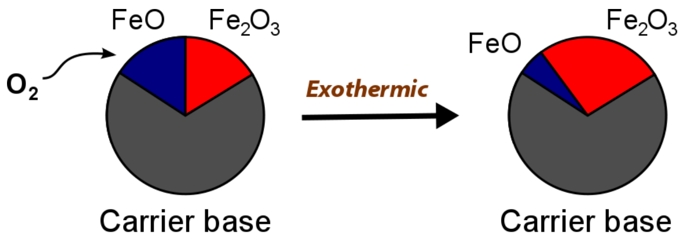
Ilmenite Carrier

- Primarily consists of
  - ilmenite ($FeTiO_3$)
  - rutile (TiO_2)
  - hematite (Fe_2O_3)
- d_{50} of 156 microns
- Oxygen carrying capacity: 3.3 wt% of oxidized particle weight



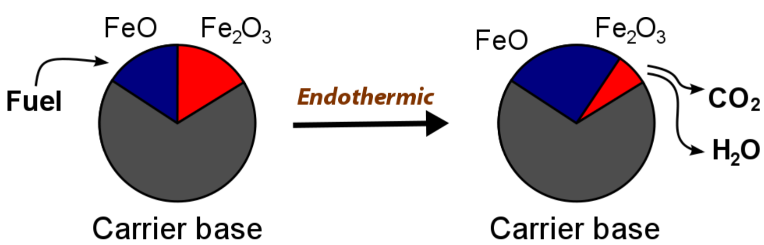
Ilmenite chemistry

Oxidation (exothermic)



$$4FeO + O_2 \rightarrow 2Fe_2O_3$$

Reduction (endothermic)



$$4Fe_2O_3 + CH_4 \rightarrow 8FeO + CO_2 + 2H_2O$$

$$Fe_2O_3 + H_2 \rightarrow 2FeO + H_2O$$

$$Fe_2O_3 + CO \rightarrow 2FeO + CO_2$$

Rates from Abad et al (2001)

CLC subset models

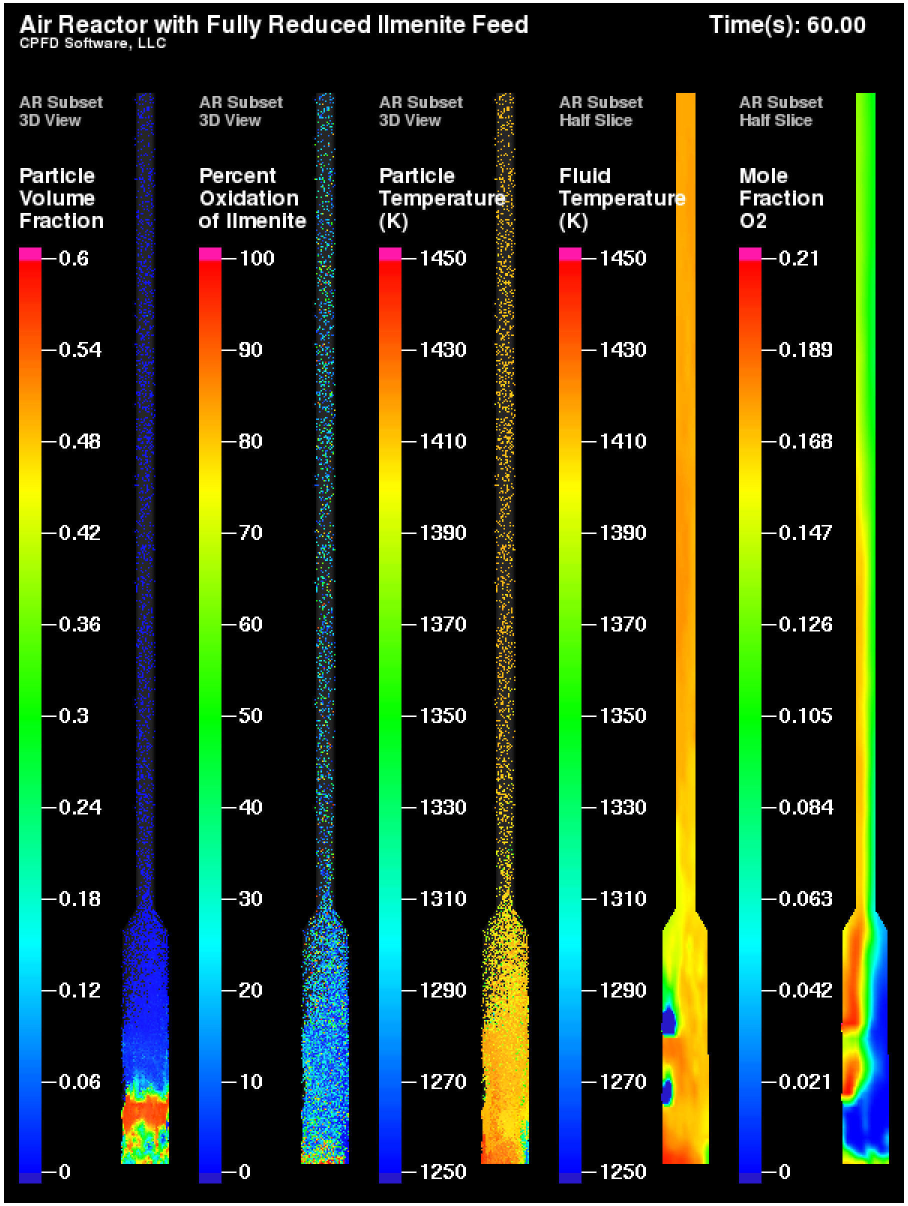
- Apply ilmenite chemistry
  - air reactor subset model
  - fuel reactor subset models

Air reactor subset

- Ilmenite enters air reactor completely reduced

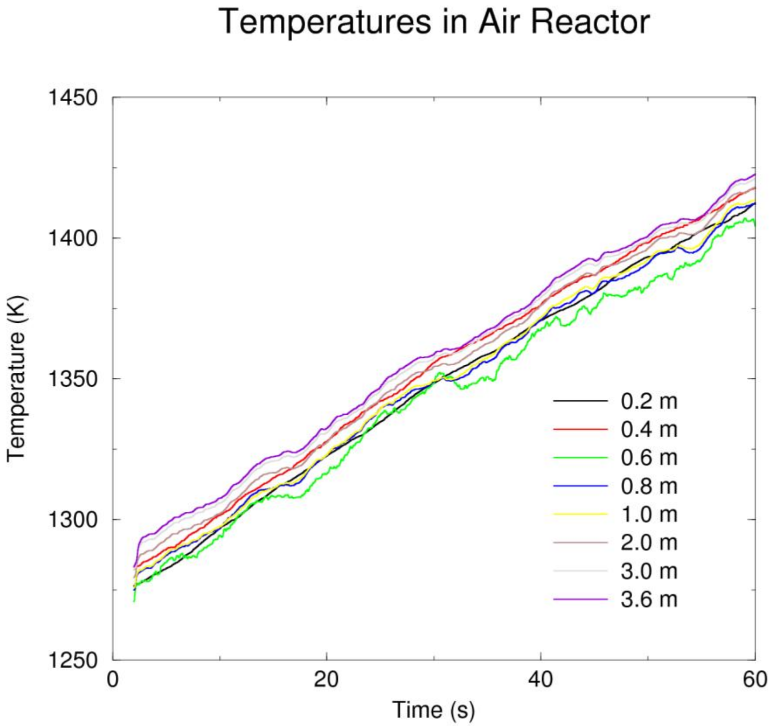
$$\text{Percent Oxidation} = \frac{w_{Fe_2O_3}}{0.307} \times 100$$

- Max Fe_2O_3 on particle: 30.7 wt%

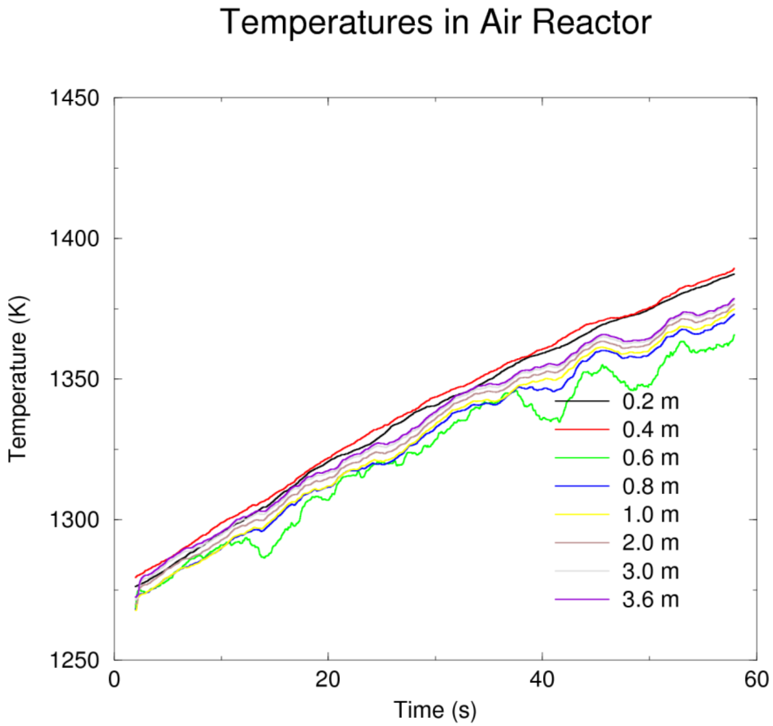


Oxidation level of ilmenite feed

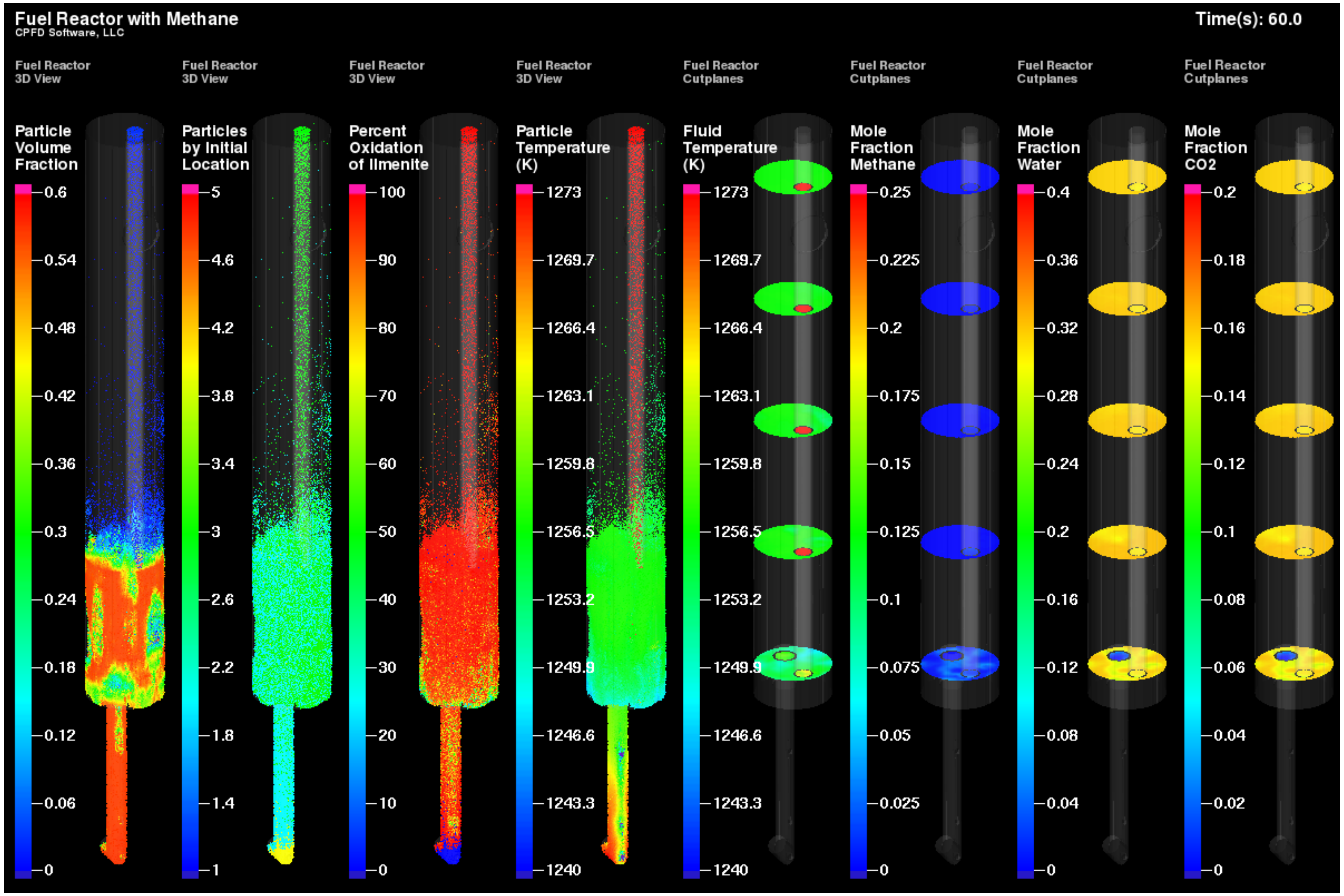
- Ilmenite enters air reactor **unoxidized**



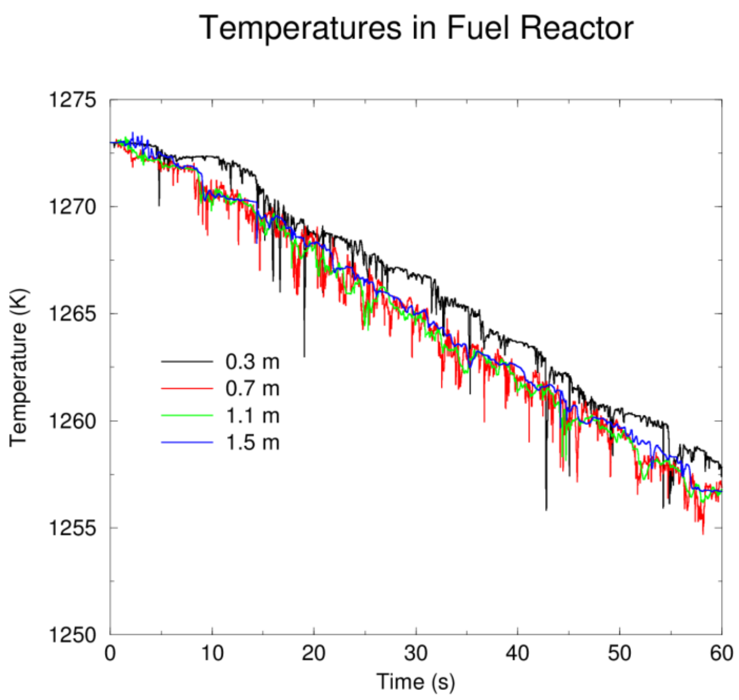
- Ilmenite enters air reactor **65%** oxidized

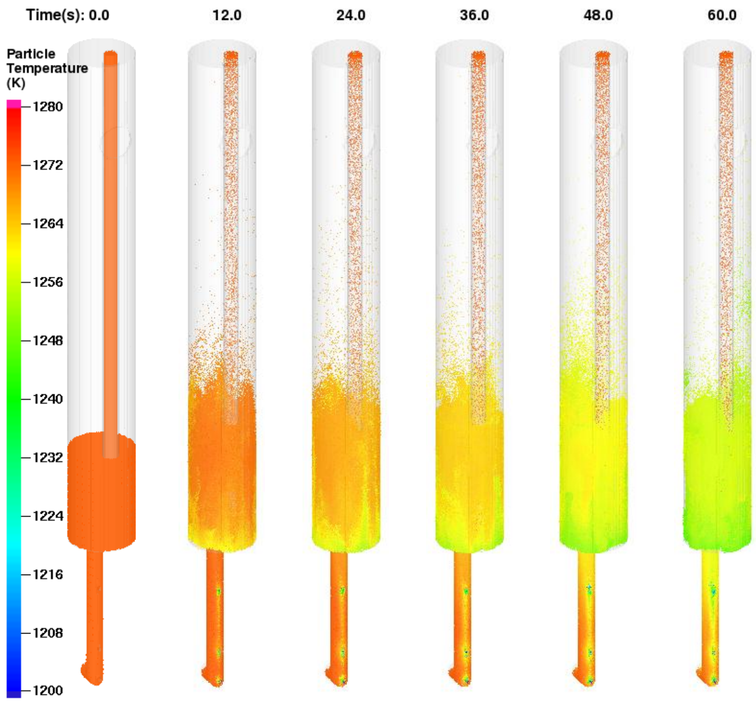


Fuel reactor subset with methane



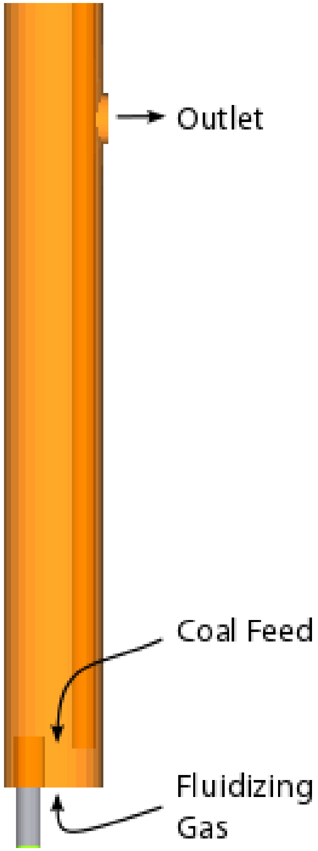
Temperatures in Fuel Reactor with methane





Coal chemistry

- **Coal devolatilization**
  - Temperature-dependent release of methane, carbon dioxide, carbon monoxide, water
  - Included particle swelling effects
- **Coal drying**
  - Mass transfer limited release of moisture from particle. Equilibrium between solid and gas phase.
- **Gasification of carbon**
  - Steam gasification producing carbon monoxide, hydrogen
  - CO_2 gasification producing carbon monoxide
- **Water-gas shift reaction**
- **Ilmenite reduction reactions**
  - Reduction reactions of Methane , Hydrogen , Carbon monoxide



Coal particle properties

- Initial particle density: 1333 kg/m^3
- 50 micron – 150 micron particle diameter
- Heat of combustion: 32 MJ/kg

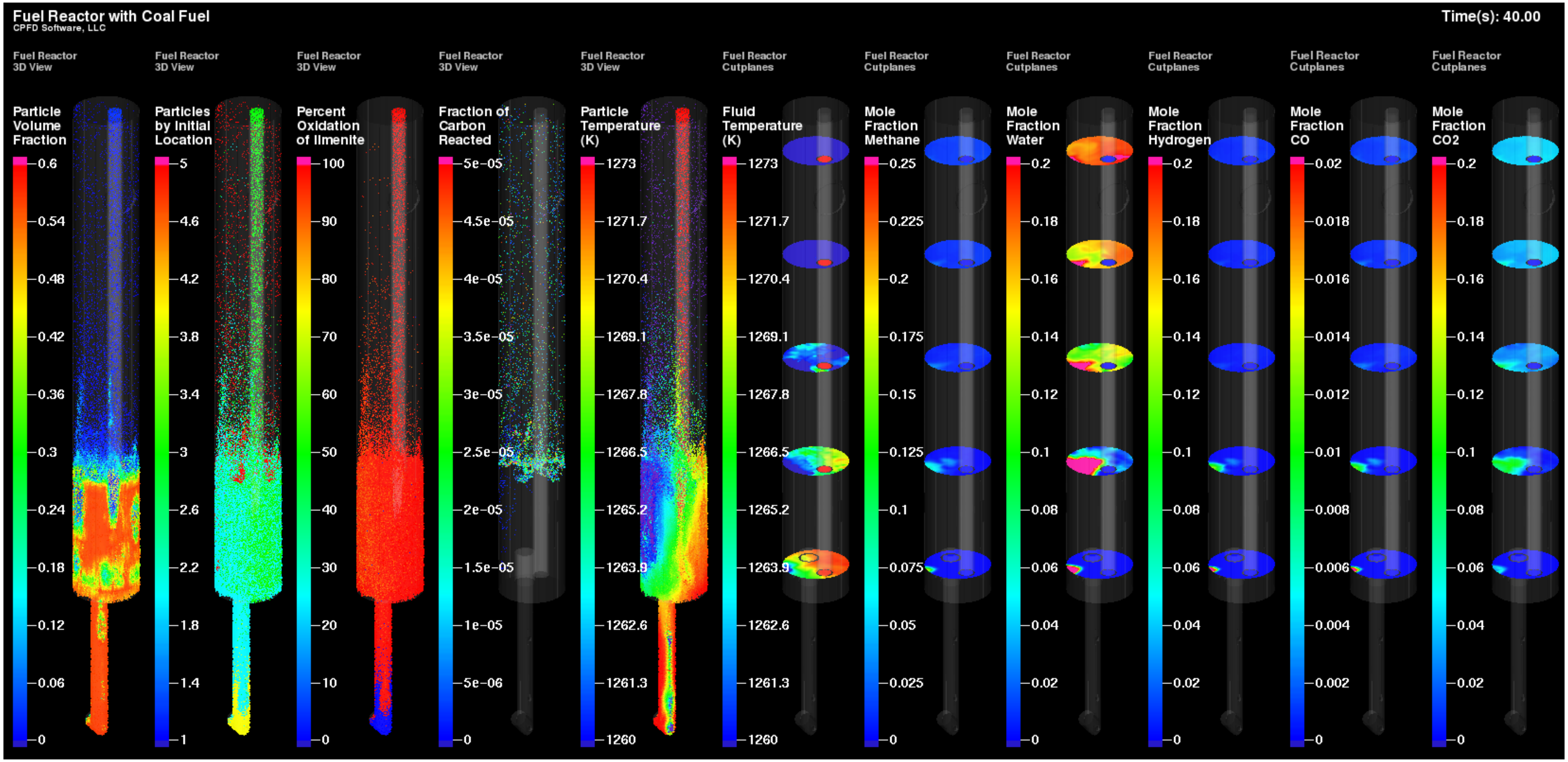
Initial coal composition

Component	Composition (wt%)	Density (kg/m^3)
Char	51%	2150
Volatile Organics	34%	815
Ash	10%	2200
Moisture	5%	1000

Released Gases

Component	Composition (wt%)
Methane	66.8%
Carbon monoxide	24.4%
Water	5.9%
Carbon dioxide (gas)	2.8223%
Carbon dioxide (trapped)	0.0777%

Coal particle subset model

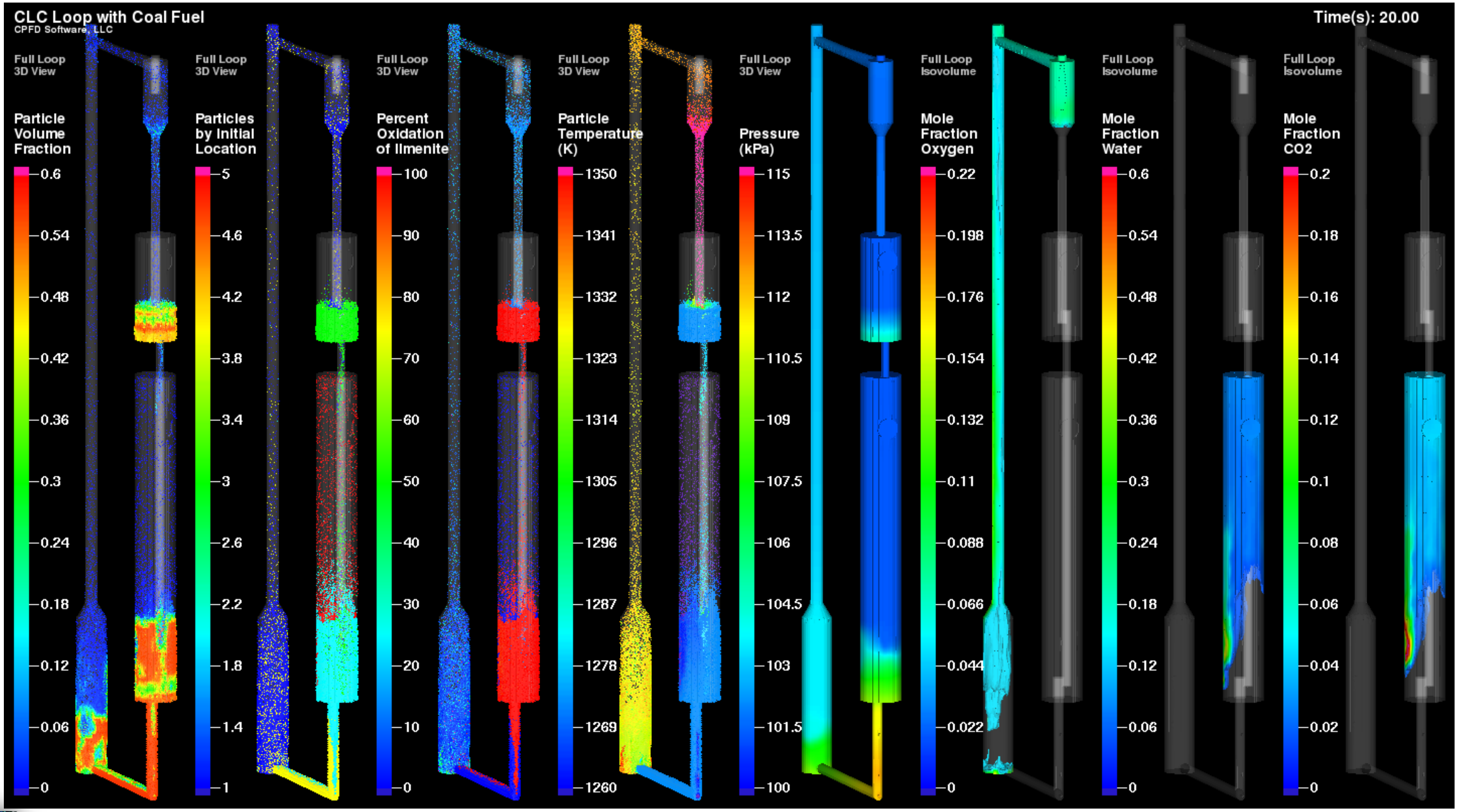


Full CLC simulation with coal

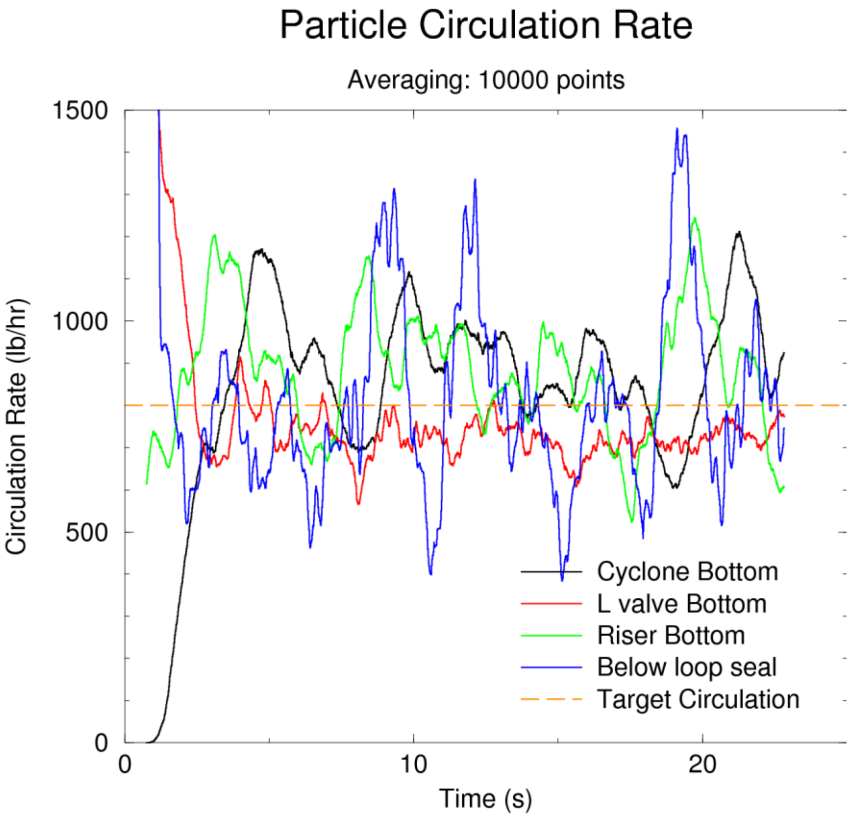
- Apply ilmenite chemistry and coal chemistry to loop

- Coal feed is 2.7 lb/hr at 298K

Full CLC loop simulation



Full CLC loop simulation



- Simulated circulation rate is close to target rate of 800 lb/hr

Conclusions

- Full reacting chemical looping combustion system was modeled in 3D
- Model highlights
  - Composition of solid ilmenite carrier was tracked on each computational particle in model
  - Oxidation/reduction of ilmenite is modeled using particle level chemistry
  - Coal particles were modeled as a fuel source, including devolatilization, moisture release, and gasification reactions
- Tool for future design and optimization work

Acknowledgements

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