

Simulation of Incineration of Waste Generated from Cleanup following Chemical/Biological Incidents

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Outline

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 - EPA's pilot-scale Rotary Kiln Incinerator Simulator (RKIS)
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 - WTE Stoker
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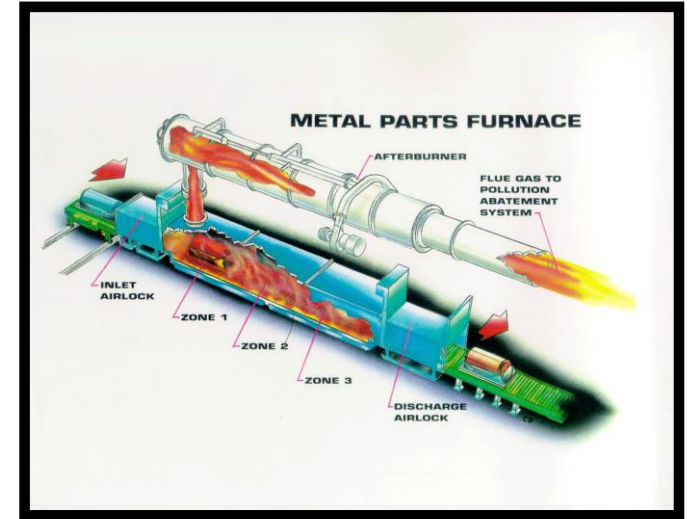
Motivation for Configured Fireside Simulator (CFS)

- Incineration is a likely treatment technology to destroy residual chemical and biological (CB) threat agents from a contamination incident
 - On-site
 - Off-site
- Substrates on which these agents will be bound have a profound impact on the behavior of the waste streams in the incinerators.
- Full-scale testing may not be able to encompass the variety of materials and agents.
- Logistical and public perception issues may make it very difficult or impossible to do testing at a specific incineration facility with the specific types of materials that would be containing these trace level contaminants.



History of CFS Software

- The Configured Fireside Simulator (CFS)
 - Originally developed for the Department of Defense to evaluate operations of the chemical demilitarization incinerators processing the US's chemical warfare agent stockpile
- Destruction kinetics developed for US warfare agent stockpile
 - GB, VX, HD, H, HT

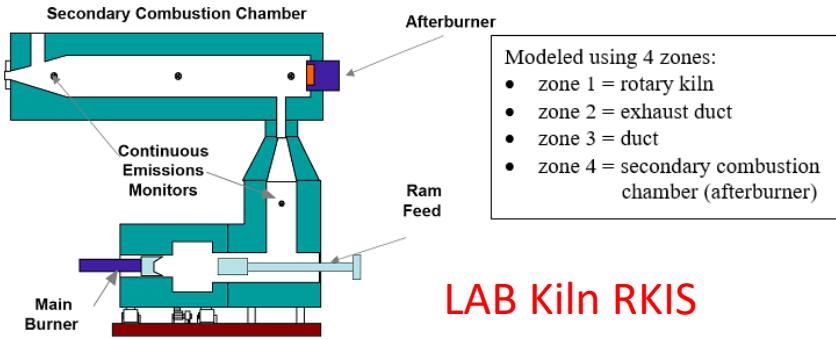


CFS Software for EPA

- Adapted to provide for the ability to run “what if” scenarios of waste streams contaminated with CB agents
 - EPA’s pilot-scale Rotary Kiln Incinerator Simulator (RKIS)
 - Three commercial incinerators based on design criteria for actual operating facilities
 - Medical/Pathological Waste Incinerator
 - Hazardous Waste Burning Rotary Kiln
 - Waste-to-Energy Stoker type combustor.
- CFS uses chemical kinetic data for destruction of chemical warfare agents
- Added biological agent destruction kinetic data derived from bench- and pilot-scale experiments performed at EPA’s Research Triangle Park, NC facility
 - Also a generic agent Arrhenius destruction input has been added

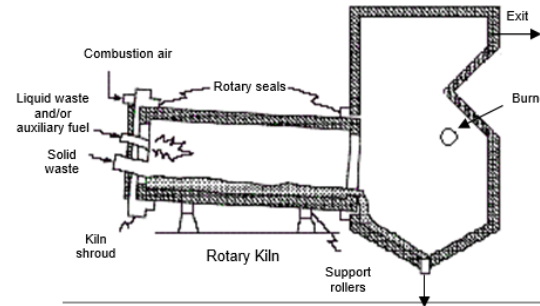


Incinerators in the CFS



LAB Kiln RKIS

Commercial Kiln



Schematic of hazardous waste kiln incinerator.

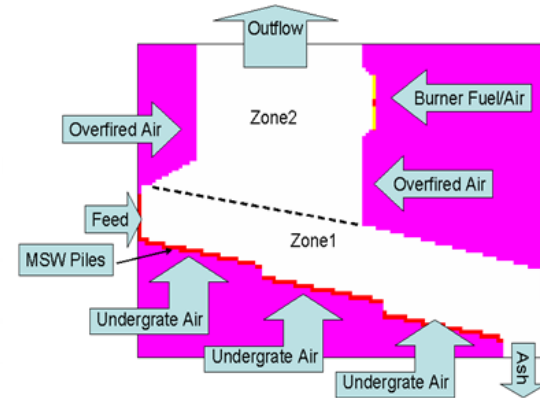
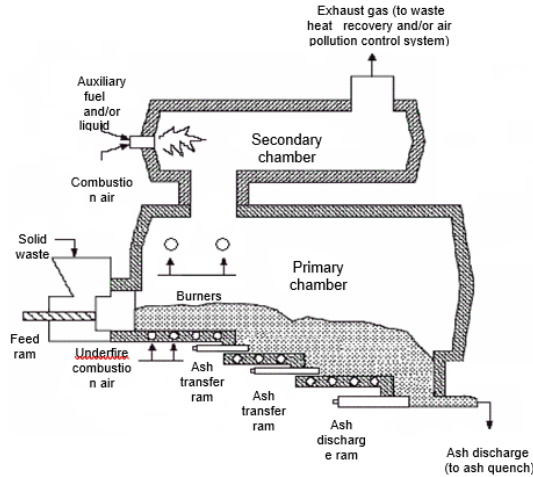
- Modeled using 4 zones:

 - zone 1 = rotary kiln
 - zone 2 = bottom - secondary combustion chamber
 - zone 3 = middle - secondary combustion chamber
 - zone 4 = top - secondary combustion chamber

Medpath

- Modeled using 2 zones:

 - zone 1 = primary chamber
 - zone 2 = secondary chamber (afterburner)

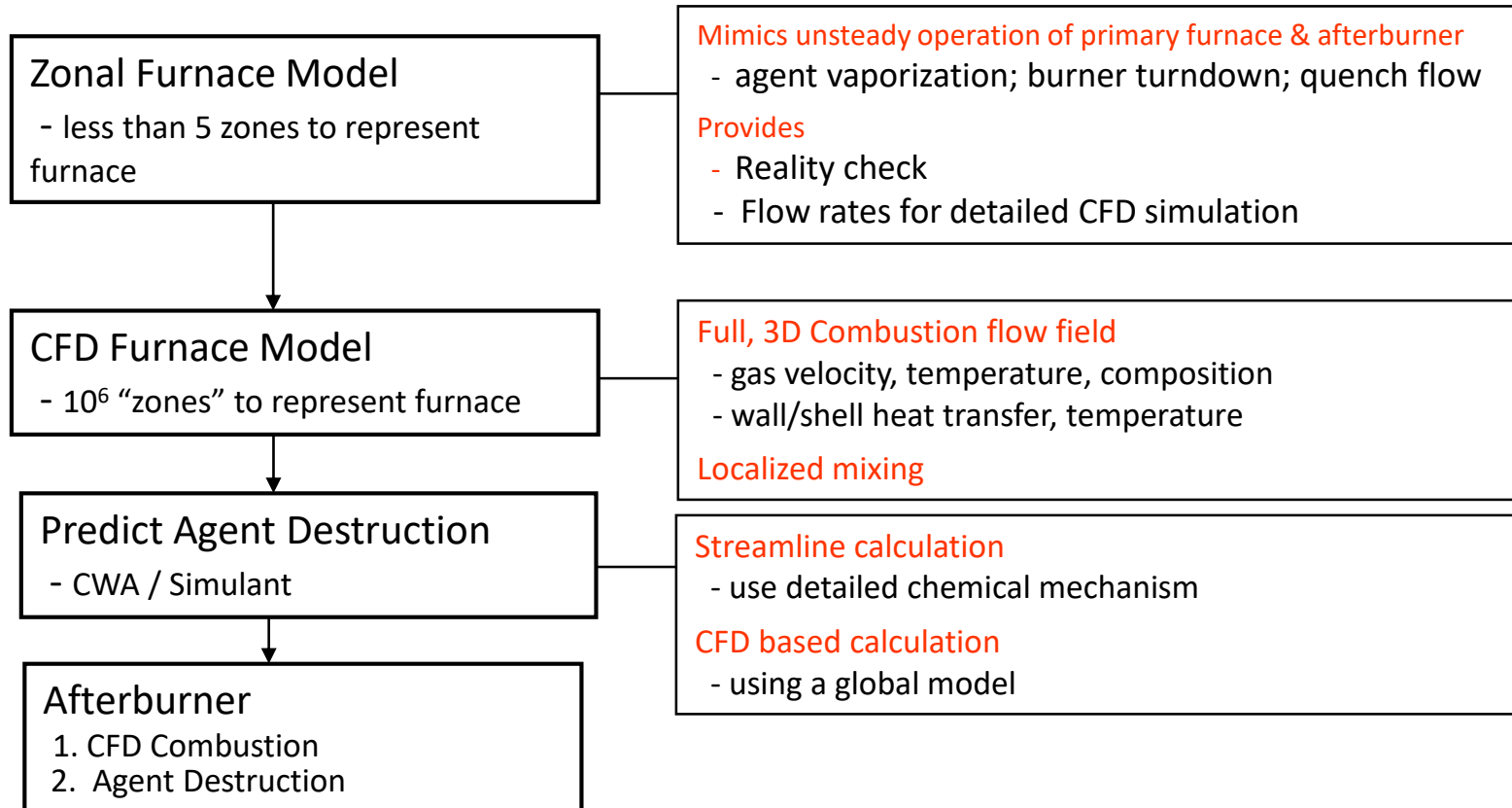


- Modeled using 2 zones:

 - zone 1 = below OFA
 - zone 2 = OFA and above

WTE Stoker Incinerator

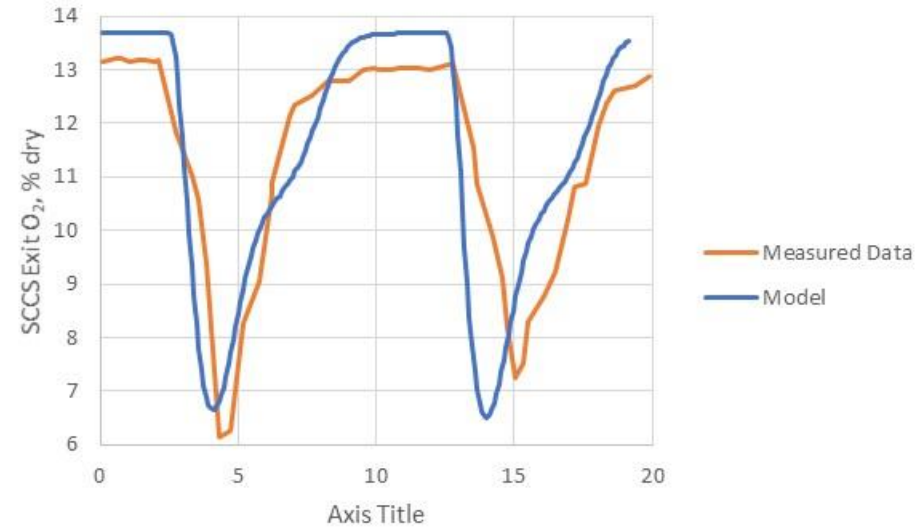
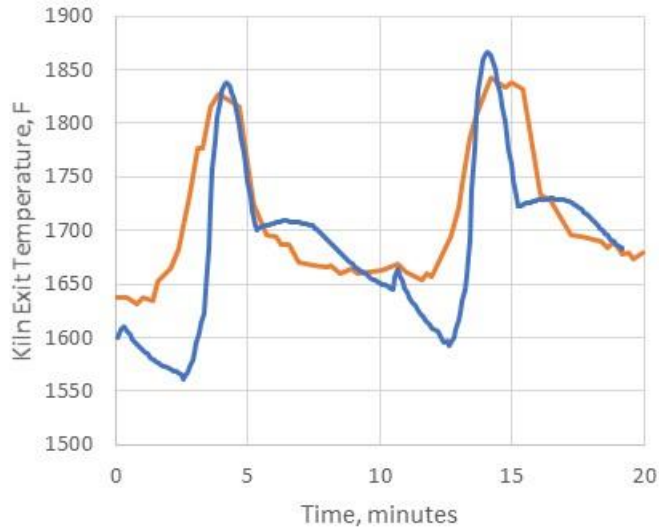
Incinerator Modeling Approach



Transient Zonal Incinerator Model

- Solve a set of Ordinary Differential Equations (ODEs)
 - Gas (Furnace)
 - Mass, Enthalpy, Material
 - Contaminated Substrate Matrix (Bundle)
 - Discretized to capture gradients of temperature, material
- Gas Approach
 - One control volume for each zone
- Equilibrium at each time step
 - Enthalpy, elemental composition => Temp., X_{species}
- Runge-Kutta integration with time step control

Transient Model RKIS Results



Incinerator Model

Zonal Furnace Model

- 3 (4) zones to represent furnace

Mimics operation of primary furnace & afterburner

- agent vaporization; burner turndown; quench flow

Provides

- Reality check
- Flow rates for detailed CFD simulation

CFD Furnace Model

- 10^6 "zones" to represent furnace

Full, 3D Combustion flow field

- gas velocity, temperature, composition
- wall/shell heat transfer, temperature

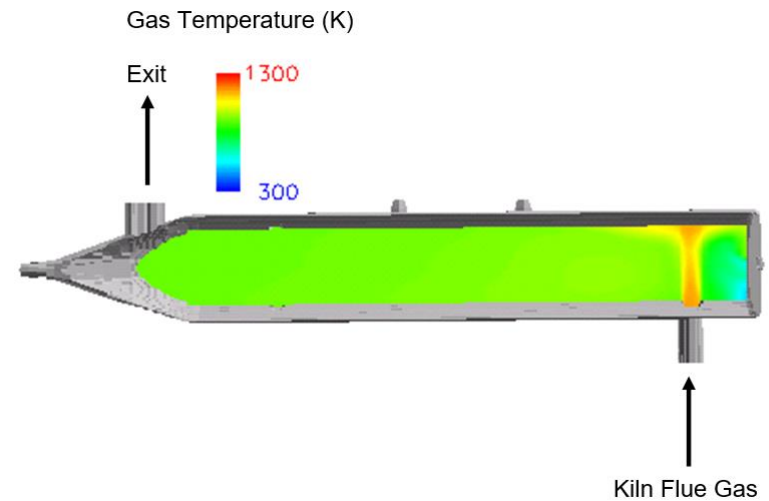
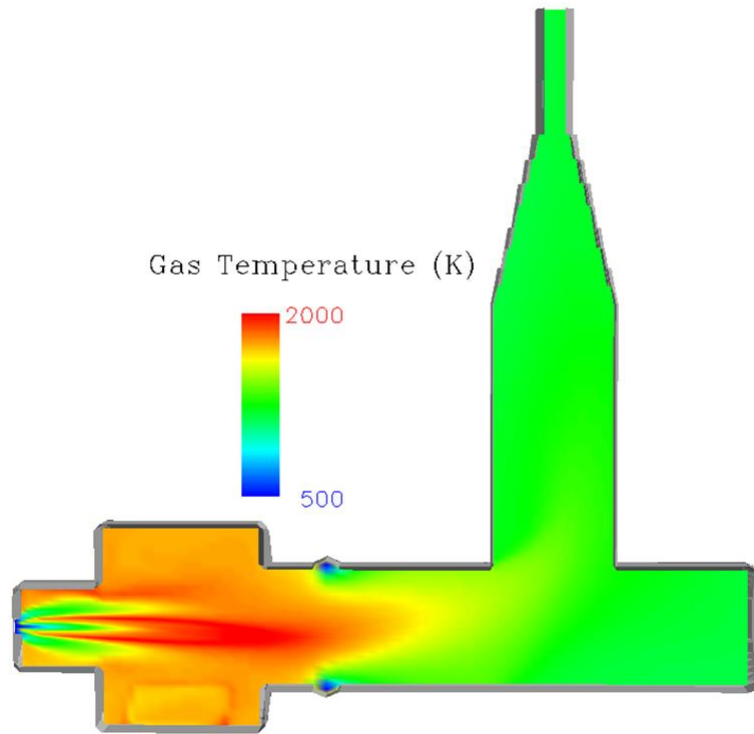
Localized mixing

CFD Model

- In House Code BANFF
- Full Equilibrium Chemistry
 - “Mixed is burnt” assumption
 - Good assumption for combustion flow field
- Major species, heat release, flow patterns
- Only need thermodynamic data
- Inadequate when kinetics are important
 - Need kinetics to predict agent destruction, NO_x , Metals, PICs

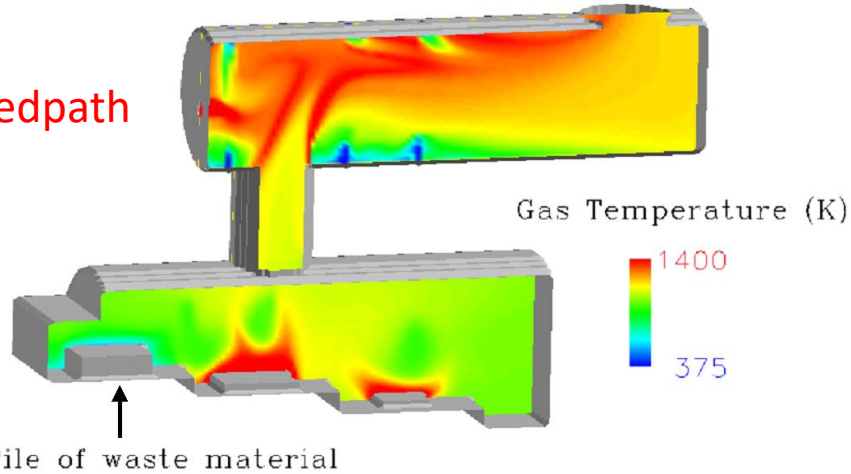


RKIS Gas Temperature Distribution

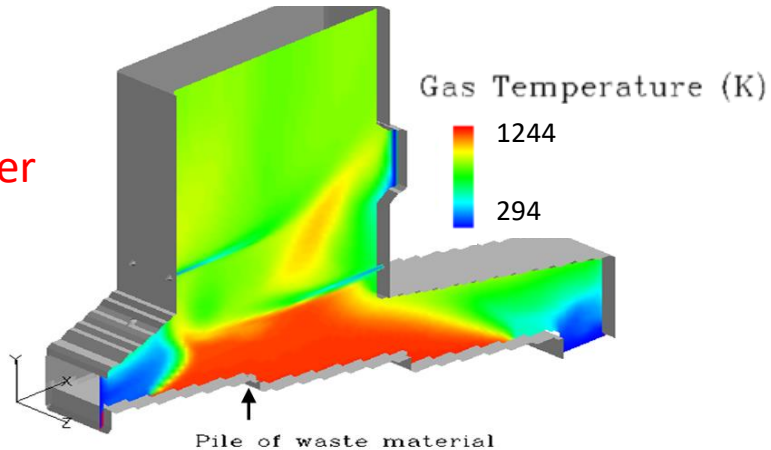


Gas Temperature Distribution

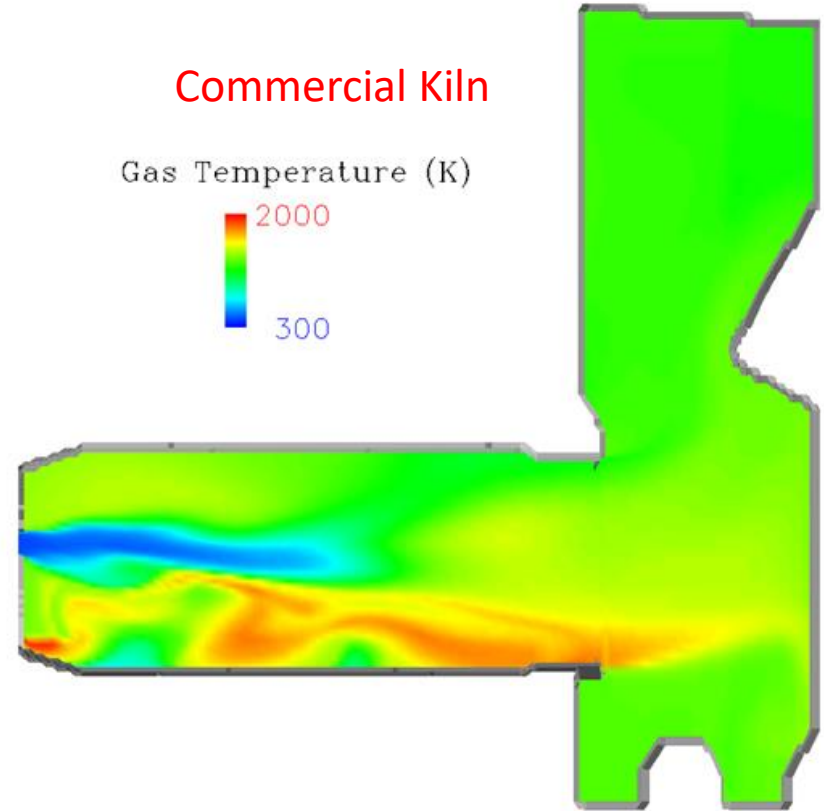
Medpath



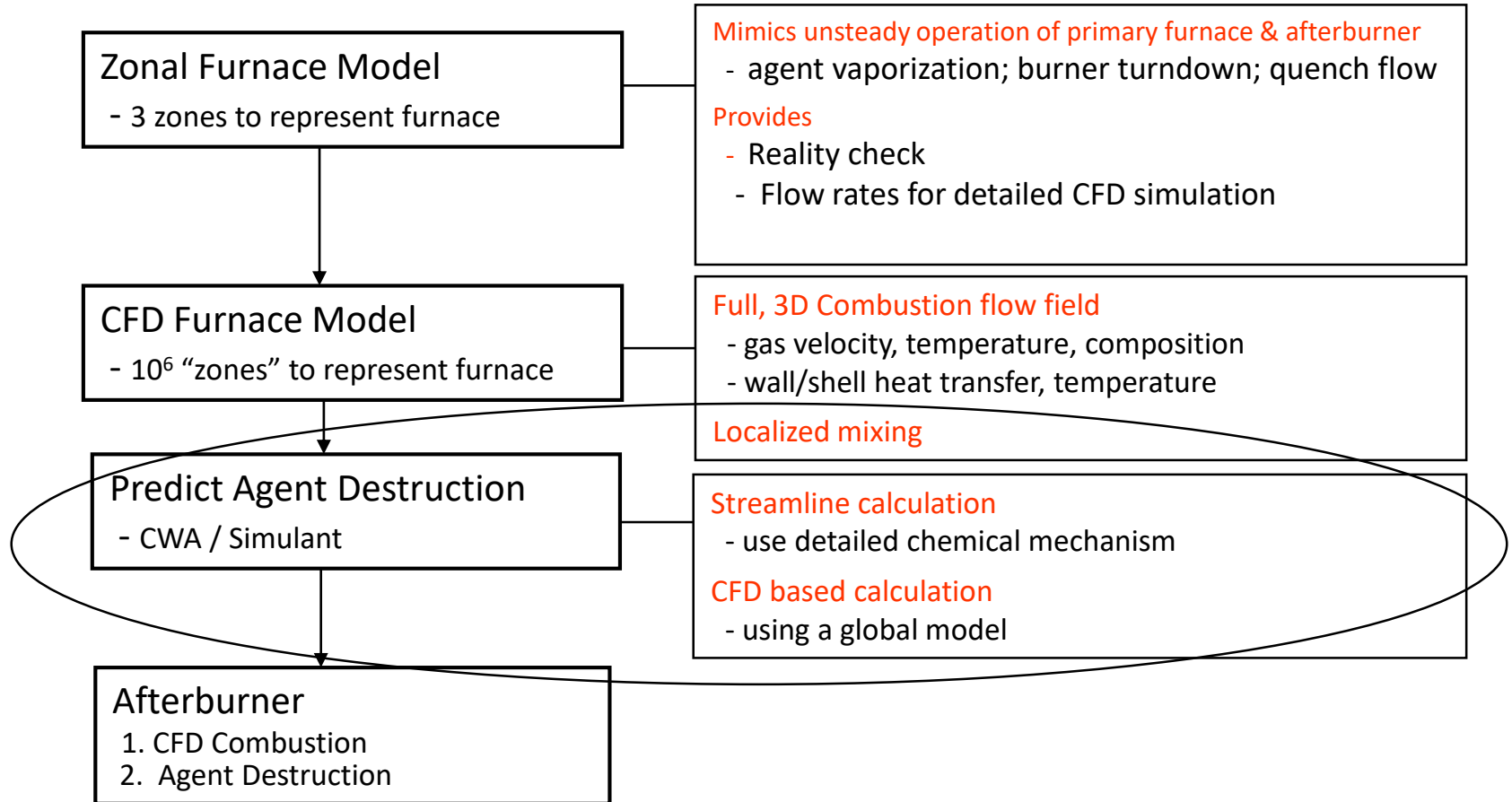
WTE
Stoker



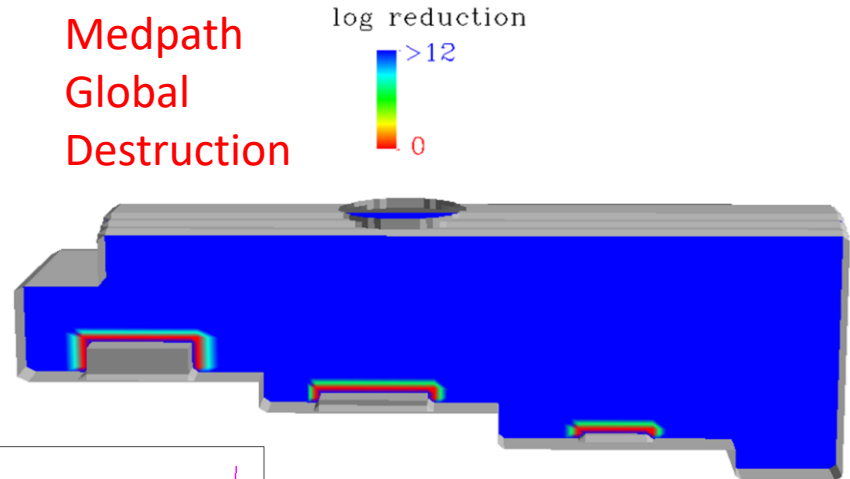
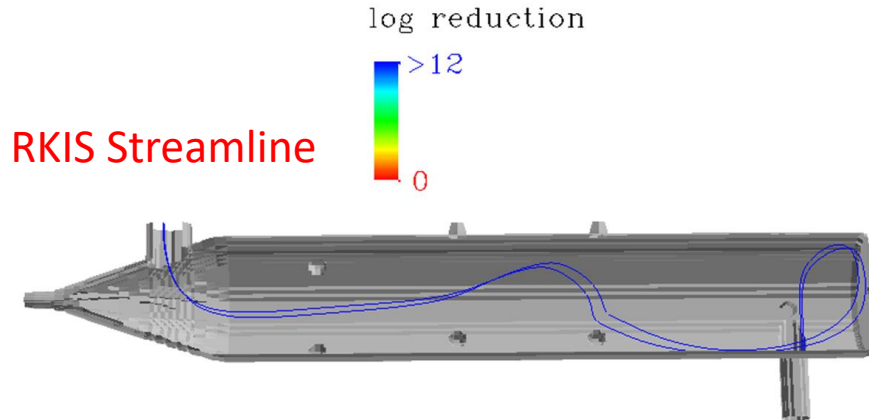
Commercial Kiln



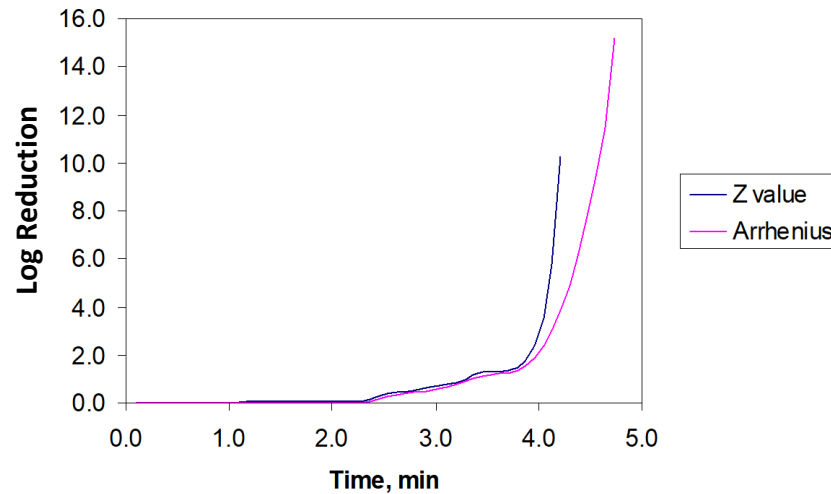
Agent Destruction



Agent Destruction



RKIS Bio Agent
Destruction in
Substrate
(Bundle)



CFS Added Capabilities

- Multiple Feed types
 - Commercial Kiln Model allows for different material at each feed event.
 - Medpath and Stoker feed defined from a set of different materials.

The screenshot displays the 'Bundle' configuration window in the transientCom_0 software. The window title is 'transientCom_0' and it has standard window controls (minimize, maximize, close). The interface is divided into several sections:

- Navigation:** 'Zones', 'Natural Gas', 'Bundle', and 'Bundle (cont.)' tabs are visible at the top.
- Bundle Configuration:** 'Working Bundle Type: 1' and 'Number of Bundle Types: 1' are shown in a dropdown menu.
- General Properties:** A table of input fields for material properties:

{Number of Pieces Per Feed}	223
{Agent Mass Fraction}	0.0001
{Density (kg/m ³)}	534.0
{Conductivity (W/mK)}	0.6
{Specific Heat (J/kg-K)}	835.0
{Furnace view factor*bundle surface emissivity}	0.2
{Critical moisture mass fraction}	0.08
- Length (m):** Three input fields for dimensions:

{X Dimension}	0.3
{Y Dimension}	0.075
{Z Dimension}	0.075
- Number of Nodes:** Three input fields for node counts:

{X Dimension}	3
{Y Dimension}	3
{Z Dimension}	3
- Bio Destruction:** A section with two input fields and two radio buttons:

A or C, 1/s	30.01
E/R or Z, K	3568.3
<input checked="" type="radio"/> Arrhenius	
<input type="radio"/> Z Value	

Only apply when agent is BIO
- Buttons:** 'Save Bundle', 'Load Bundle', 'Help', and 'Execute' are located at the bottom of the window.

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