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ADVANCED CFD MODELING FOR GASIFICATION RESEARCH AND DEVELOPMENT

VLADIMIR AGRANAT, SERGEI ZHUBRIN and MASAHIRO KAWAJI

Department of Chemical Engineering and Applied Chemistry
University of Toronto
vladimir.agranat@utoronto.ca, kawaji@chem-eng.utoronto.ca
and
Applied Computational Fluid Dynamics Analysis (ACFDA)
Thornhill, Ontario
http://www3.sympatico.ca/acfda, acfda@sympatico.ca,

Overview

- Introduction: gasification R&D and multiphase Computational Fluid Dynamics (CFD)
- Governing equations and general-purpose CFD codes (PHOENICS, FLUENT, CFX, etc.)
- Advanced CFD sub-models for gasification R&D
- Multiphase CFD capabilities at U of T and ACFDA
- Recent R&D Projects: GRAD CFD, GLASS and COFFUS related studies
- Conclusions

Introduction: gasification R&D and multiphase CFD

- **Solid/liquid fuel gasification and combustion in a furnace:**
  - Multi-physics: multiphase flow, turbulence, phase change, homogeneous and heterogeneous combustion, radiation
  - Multi-scale: small particles and large furnace dimensions
  - Expensive experimentation for optimal furnace design
  - Need for CFD predictions (faster and cost-effective design)
- **Multiphase CFD capabilities:**
  - Commercial general-purpose CFD codes (PHOENICS, FLUENT, CFX, etc.) - framework for CFD analyses
  - Advanced customized CFD sub-models for gasification R&D
  - CFD predictions as scientific basis for optimal furnace design
  - Cost-effective and reliable design tool (effect of furnace geometry and input conditions)
  - Safety and environmental analyses

Governing equations and general-purpose CFD codes

- Various commercially available CFD software packages (PHOENICS, FLUENT, CFX, etc.) are equipped with multiphase flow capabilities
- Governing equations include:
  - conservation equations for mass, momentum and energy for each phase,
  - constitutive equations (linkage between phases)
  - turbulence model equations,
  - chemical kinetics (homogeneous and heterogeneous reactions)
  - equations for radiative heat transfer
- **Need for advanced customized models for gasification R&D**
  - Develop new sub-models for more accurate predictions
  - Validate models using experimental data
  - Apply models as cost-effective, rapid design tool

Multiphase CFD capabilities at U of T and ACFDA

- **Multiphase CFD** research group at U of T works on CFD analyses of complex industrial multiphase flow processes (chemical, energy, environmental, petroleum, etc.) including
  - Advanced cutting-edge CFD model development
  - Model validation (experimental fluid dynamics)
  - Model customization and application to challenging real-life problems
- **Research team** consists of CFD experts with 25+ years of experience in CFD R&D (both academic and industrial)
- **Products and services**:
  - Advanced customized multiphase CFD software modules for real-life industrial applications (gasification R&D, safety, design)
  - CFD consulting services
  - CFD training and support
- **Approach:**
  - **Provide complete set of model development, validation and customization**

Recent R&D projects: GLASS, GRAD CFD and COFFUS related modules

- **Advanced CFD models (developed over the last 7 years):**
  - **GLASS, Gas-Liquid flow Analysis and Simulation Software,** for analyses of complex gas-liquid flows and heat/mass transfer in complicated geometries (no limitations on flow regime):

    http://www3.sympatico.ca/acfda/Docs/ASME2006-98355.pdf
  - **GRAD CFD** module, for advanced CFD modeling of Gas Release and Dispersion (safety and environmental):

    http://www3.sympatico.ca/acfda/Docs/Paper_NATO_2006_Final.pdf
  - **Advanced CFD modeling of coal/wood/biomass gasification and combustion** (extensions of COFFUS in PHOENICS):

    http://www.simuserve.com/cfd-shop/uslibr/reactive/fur-sing.htm

    http://www.cham.co.uk/phoenics/d_polis/d_applic/d_comb/coalgas/coalgas.htm

    http://www.cham.co.uk/website/new/mica/coffus.htm

GLASS case study: CFD model development for gas-liquid flows in water electrolysis systems

- Water electrolysis systems are used to produce hydrogen from water
- Computational fluid dynamics (CFD) is applied as a design tool to predict gas-liquid flows and heat/mass transfer in water electrolysis systems
- CFD models can predict:
  - 3D distributions of gas and liquid phases, their velocities, temperatures and pressure throughout entire system
  - Gas-liquid separation efficiency
  - Hydrogen gas purity
  - Electrolyte circulation rate
  - Heat and mass transfer rates
- CFD sensitivity runs allow for determination and optimization of critical design parameters
- Optimized cell stack design can be achieved rapidly and economically

GLASS case study: governing equations

Mass and momentum conservation equations of Inter-Phase Slip Algorithm (IPSA), option in commercial PHOENICS CFD software:

$$\frac{\partial}{\partial x}(\rho_i \alpha_i u_i) + \frac{\partial}{\partial y}(\rho_i \alpha_i v_i) = 0$$

$$\frac{\partial}{\partial x}(\rho_i \alpha_i u_i^2) + \frac{\partial}{\partial y}(\rho_i \alpha_i u_i v_i) = -\alpha_i \frac{\partial P}{\partial x} + F_r(u_j - u_i) + \frac{\partial}{\partial x}\left(\alpha_i \mu_{eff} \frac{\partial u_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\alpha_i \mu_{eff} \frac{\partial u_i}{\partial y}\right)$$

$$\frac{\partial}{\partial x}(\rho_i \alpha_i v_i u_i) + \frac{\partial}{\partial y}(\rho_i \alpha_i v_i^2) = -\alpha_i \frac{\partial P}{\partial y} + F_r(v_j - v_i) + \frac{\partial}{\partial x}\left(\alpha_i \mu_{eff} \frac{\partial v_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\alpha_i \mu_{eff} \frac{\partial v_i}{\partial y}\right) + F_b$$

$$F_r = 0.75 \frac{c_d \rho_L \alpha_L \alpha_G}{d_b} |V_r|$$

Fr is the friction between the two phases (gas and liquid)

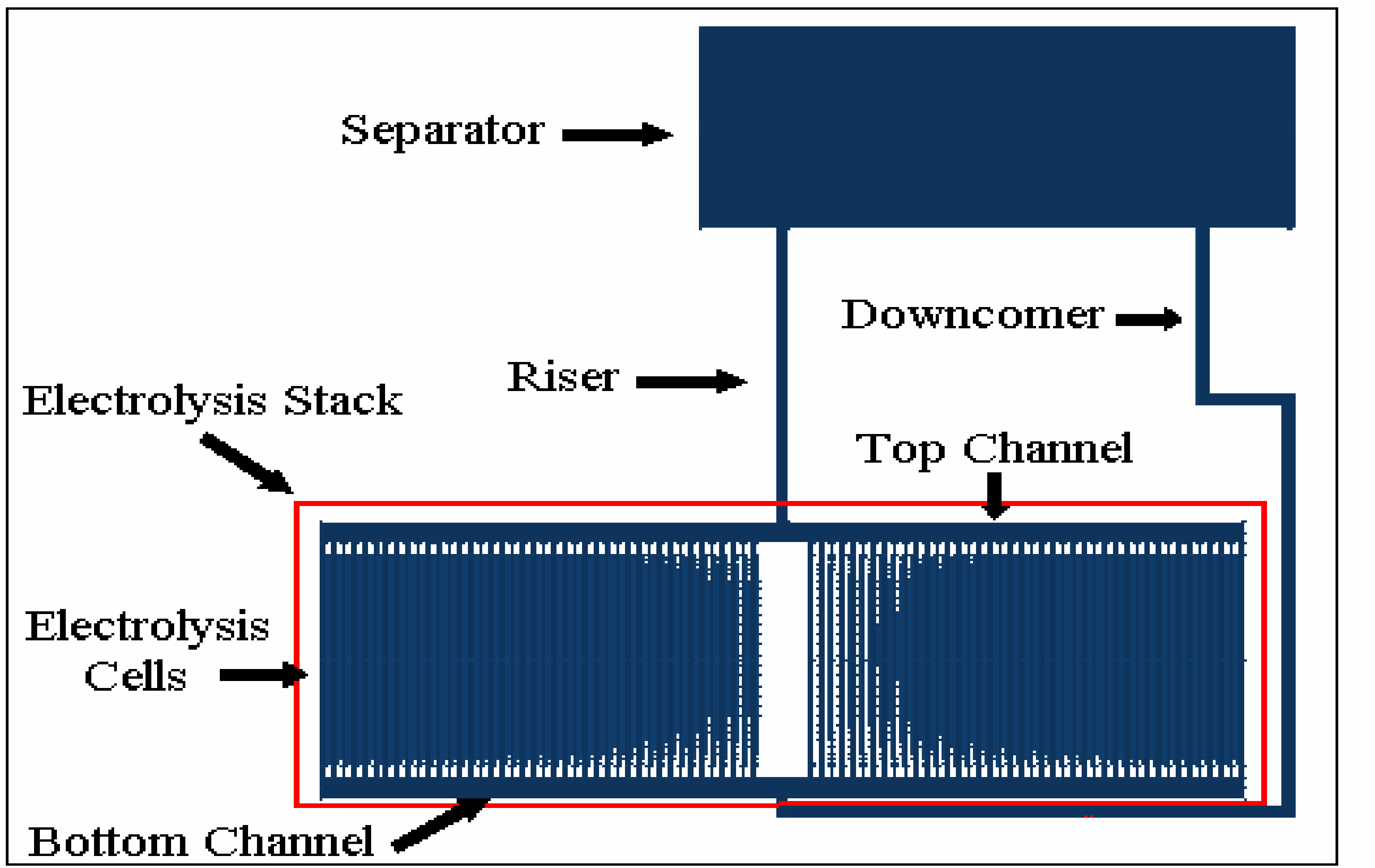
The bubble size, *db*, is an important parameter that affects the overall liquid flow rate

$$u_{GI} = \frac{1}{2} \frac{R(T + 273.15)}{P} \frac{i}{F}, F = 96487 C/mol, R = 8.314 J/molK$$

GLASS case study: advanced CFD model capabilities

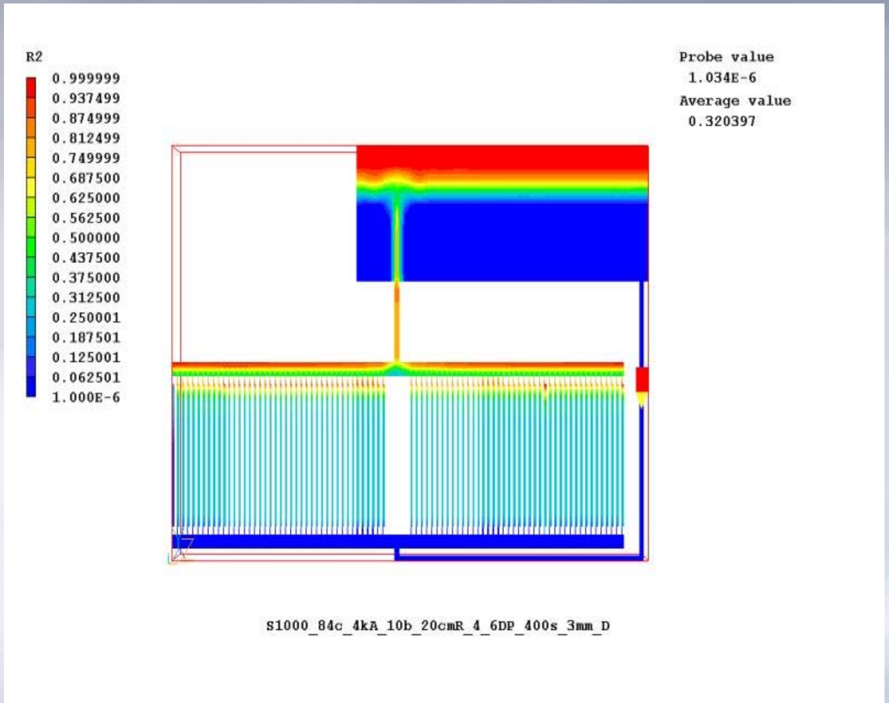
- Limitations of general-purpose CFD codes: constant bubble size, given liquid flow rate, high Reynolds turbulence, convergence issues
- No commercial CFD code is capable of modeling the whole electrolyzer (stack, separator, piping)- different flow regimes
- Advanced sub-models developed for PHOENICS: Gas-Liquid flow Analysis and Simulation Software (GLASS)
  - Two-phase turbulence
    - Effect of bubbles at low Reynolds numbers
  - Variable bubble size
    - Dependent on two-phase flow regimes
  - Phase inversion
    - Mostly liquid to mostly gas
  - Heat and mass transfer
  - Convergence promotion methods
    - Reduce computational requirements

GLASS case study: CFD geometry input



GLASS case study: CFD modeling results and validation

- Operating conditions
  - 10 bar, 70°C and 4.0 kA/m^2
  - Natural circulation with different flow regimes (from bubbly to separated)
- Output
  - 3D distributions of pressure, gas & liquid velocity components and gas & liquid volume fractions within computational domain
  - Total gas and liquid flow rates at the outlets
- Effects of current density and pressure on electrolyte flow rate and hydrogen volume fraction matched well with experimental data
  - CFD predictions and electrolyte flow measurements were within 6% at standard operating conditions



Hydrogen volume fraction, R2, in commercial electrolysis system under standard operating conditions.

GLASS validation

- GLASS is a validated CFD modeling tool for cell stack and peripherals design:
  - Validated for the entire real-life water electrolysis system (84-cell stack) at moderate and high pressures through physical experimentation
  - Predicting accurately electrolyte flow in the whole system (stack, piping, separator)
  - Predicting accurately cooling requirements in the whole system

- **Quantitatively accurate**: disagreements between the CFD predictions and electrolyte flow measurements were within 6% at a pressure of 5 bar and current densities up to 4 kA/m2
- **Qualitatively correct**: predicted effects of current density and pressure on electrolyte flow rate and hydrogen volume fraction matched well experimental data

GLASS case study: summary

- Advanced CFD models of gas-liquid flows in complex systems have been developed, validated and are being used to simulate two-phase flows in alkaline water electrolysers
- Unique modeling capabilities enable comprehensive system design:
  - Gas-liquid flow predictions for all flow regimes
  - Heat & mass transfer predictions for the whole system
  - Design capability for modules with multiple cell stacks (distributed resistance method)
- Benefits include:
  - Rapid design optimization capability
  - Reduced development time, risk and cost

GRAD CFD module: prediction of flammable gas clouds

Modeling of various flammable GRAD scenarios is based on general transient 3D conservation equations (gas convection, diffusion and buoyancy) with proper initial and boundary conditions

- 1) transient behavior of all calculated variables (pressure, gas density, velocity and flammable gas concentration)
- 2) movement of flammable gas clouds with time
- 3) safety evaluation by analyzing a flammable gas concentration iso-surface (lower flammability level (LFL)) and total volumes of flammable gas

- Three major stages in GRAD modeling:
  - 1) steady-state before-the-release simulations
  - 2) transient during-the-release simulations
  - 3) transient after-the-release simulations

- CFD framework: PHOENICS general-purpose CFD software
  - Commonly used and well validated (more than 20 years)
  - Friendly interface for incorporating GRAD sub-models
  - Various turbulence models: LVEL, MFM and k-ε variants

GRAD CFD module: governing equations

- **3D momentum equations**

$$\frac{\partial(\rho u_i)}{\partial t} + \mathrm{div}(\rho U u_i - \rho \nu_{eff}\ \mathrm{grad}\, u_i) = -\frac{\partial P}{\partial x_i} + \rho f_i, \qquad i=1,2,3$$

- **Continuity equation**

$$\frac{\partial \rho}{\partial t} + \mathrm{div}(\rho U) = 0$$

- **Flammable gas mass conservation equation**

$$\frac{\partial(\rho C)}{\partial t} + \mathrm{div}(\rho U C - \rho D_{eff}\, \mathrm{grad}\, C) = C''$$

- **Gas mixture density based on flammable gas mass concentration, *C*, or flammable gas volumetric concentration, α**

$$\rho = \frac{P}{[C R_{gas} + (1-C) R_{air}]T} \qquad \alpha = \frac{C R_{gas}}{C R_{gas} + (1-C) R_{air}}$$

- **Effective viscosity and diffusivity**

$$\nu_{eff} = \nu_l + \nu_t,\ D_{eff} = \nu_l / \mathrm{Pr}_l + \nu_t / \mathrm{Pr}_t \qquad \nu_l = [\alpha \rho_{gas} \nu_{gas} + (1-\alpha) \rho_{air} \nu_{air}] / \rho$$

Advanced GRAD CFD model features

- **Dynamic Boundary Conditions at Release Orifice:**
  - Transient choked mass flow rate

$$\dot{m}(t) = -V\frac{d\rho}{dt} = \rho(t)u(t)A \approx \dot{m}_0 e^{-\frac{C_d A}{V}t\sqrt{\gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}RT}},$$

  - Initial choked mass flow rate

$$\dot{m}_0 = C_d A\sqrt{\rho_0 P_0 \gamma\left(\frac{2}{\gamma+1}\right)^{\frac{\gamma+1}{\gamma-1}}}$$

- **Real Gas Law Properties:**
  - Abel-Noble Equation of State for hydrogen

$$z_{H_2} = \frac{P}{\rho_{H_2} R_{H_2} T} = \left(1 - \frac{\rho_{H_2}}{d_{H_2}}\right)^{-1} \qquad z_{H_2} = 1 + \frac{P}{d_{H_2} R_{H_2} T}$$

  - NIST data for methane, propane …
- **Turbulence Model Settings:**
  - LVEL model, k-ε model, k-ε RNG model, k-ε MMK model and MFM
- **Local Adaptive Grid Refinement (LAGR)**
  - Iterative technique, accurate capture of flammable cloud behaviors near the release location and large gradient regions

GRAD CFD module validation matrix

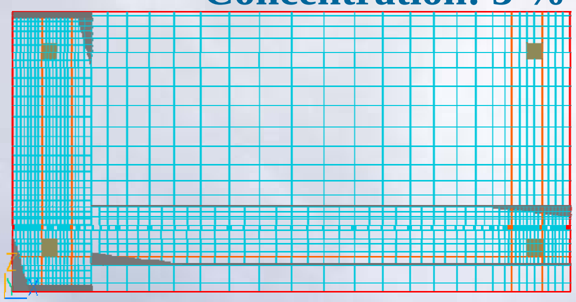
Validation, calibration and enhancement of GRAD CFD module capabilities for simulation of HYDROGEN releases and dispersion using available experimental databases

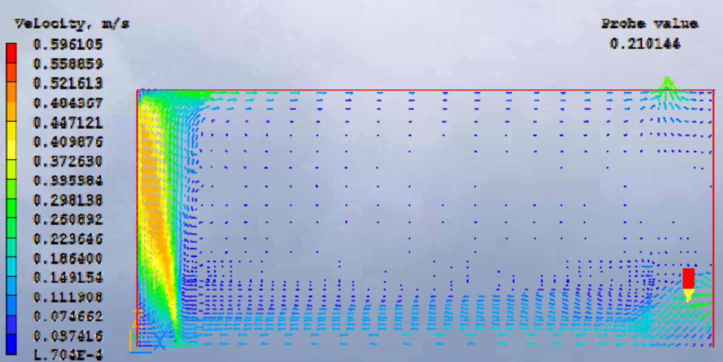
Case No.	Validation Case Name	Conditions			
		Domain	Leak Type	Process	Available Data
1	Helium jet	Open	Vertical	Steady	Velocity, concentration, turbulence intensity
2	H_2 jet		Horizontal	Transient	Concentration
3	INERIS jet			Steady	Concentration
4	Hallway end	Semi-enclosed	Vertical	Transient	Concentration
5	Hallway middle			Transient	Concentration
6	Garage			Transient	Concentration
7	H_2 vessel	Enclosed		Transient	Concentration

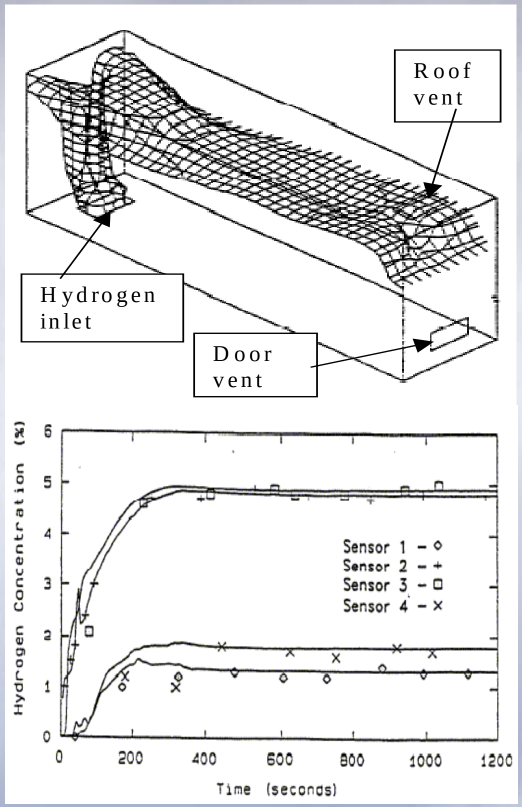
GRAD CFD module validation:

HYDROGEN SUBSONIC RELASE IN A HALLWAY

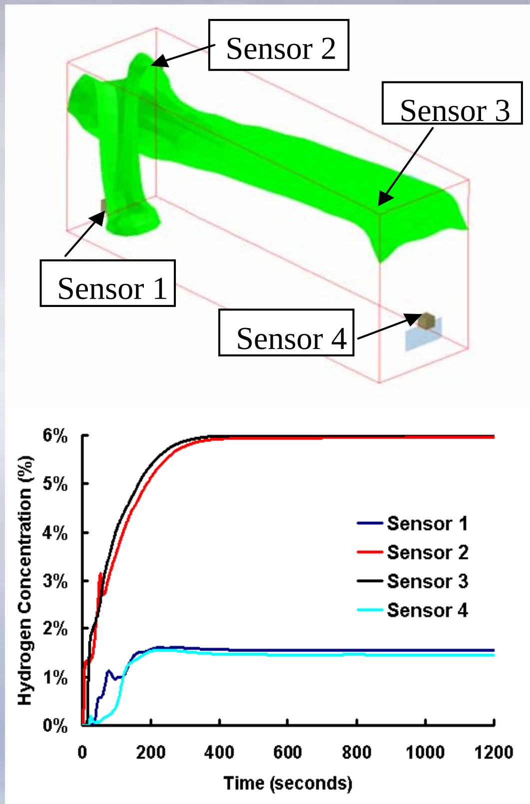
- **Concentrations at four sensors for 20 min. duration**
  - **Domain: 2.9 m × 0.74 m ×1.22 m**
  - **Grid size: 36 × 10 × 18**
  - **H_2 leak rate: 2 SCFM (0.944 m^3/s)**
  - **Duration: 20 min**
  - **Concentration: 3 % iso-surface**







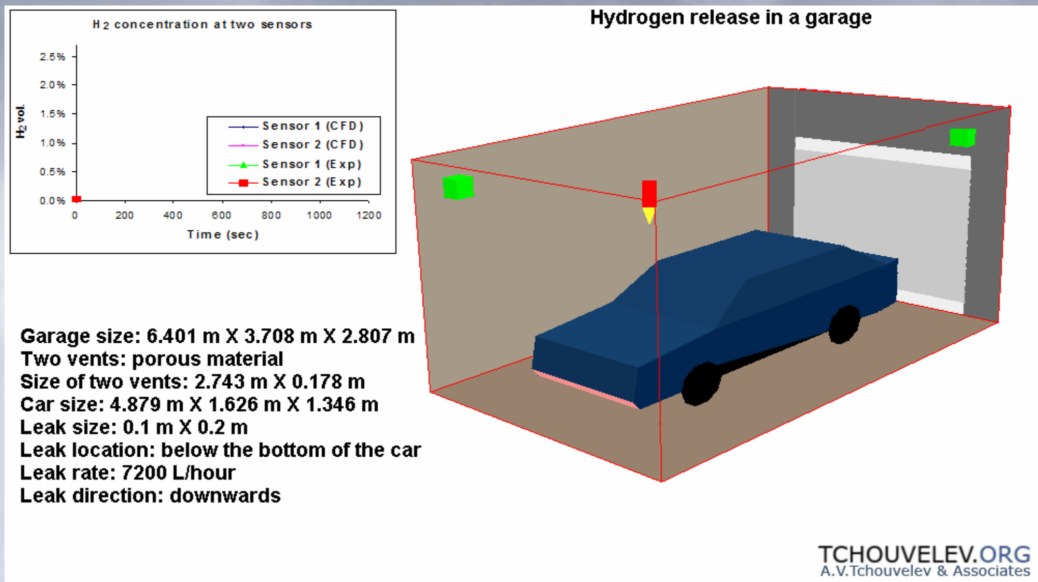
Published results



Our results

GRAD CFD module validation:

HYDROGEN & HELIUM SUBSONIC RELEASE IN A GARAGE WITH A CAR



Garage size: 6.4 m x 3.7 m x 2.8 m

Leak size: 0.1 m x 0.2 m

Two vents: porous material

Car size: 4.88 m x 1.63 m x 1.35 m

Leak rate: 7200 L/hour

Leak direction: downwards

Leak location: bottom of the car

Helium release simulated by using LAGR (local adaptive grid refinement)

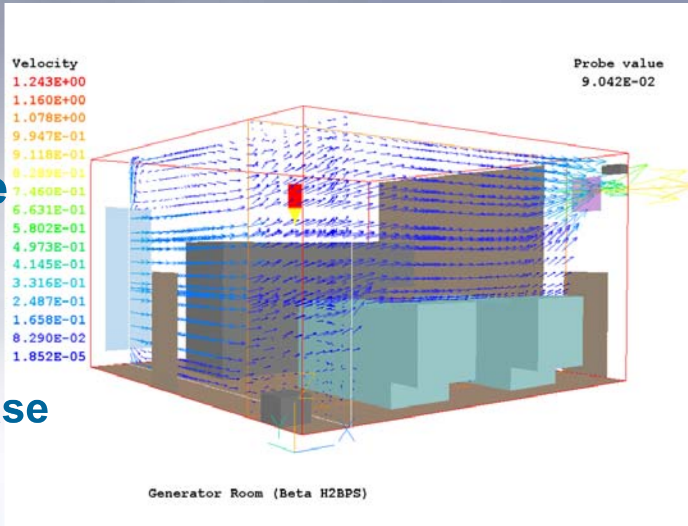
Simulations	Sensor 1	Sensor 2	Sensor 3	Sensor 4
Swain's CFD results	0.5%	2.55%	2.55%	1.0%
Initial coarse grid, 32×16×16	1.92%	2.53%	2.52%	1.94%
Adaptive refined, 39×26×24	0.98%	2.66%	2.62%	1.08%
Adaptive refined, 58×26×27	0.79%	2.70%	2.67%	1.01%

GRAD CFD module applications:

RELEASE IN A HYDROGEN GENERATOR ROOM

Before-the-Release Simulation

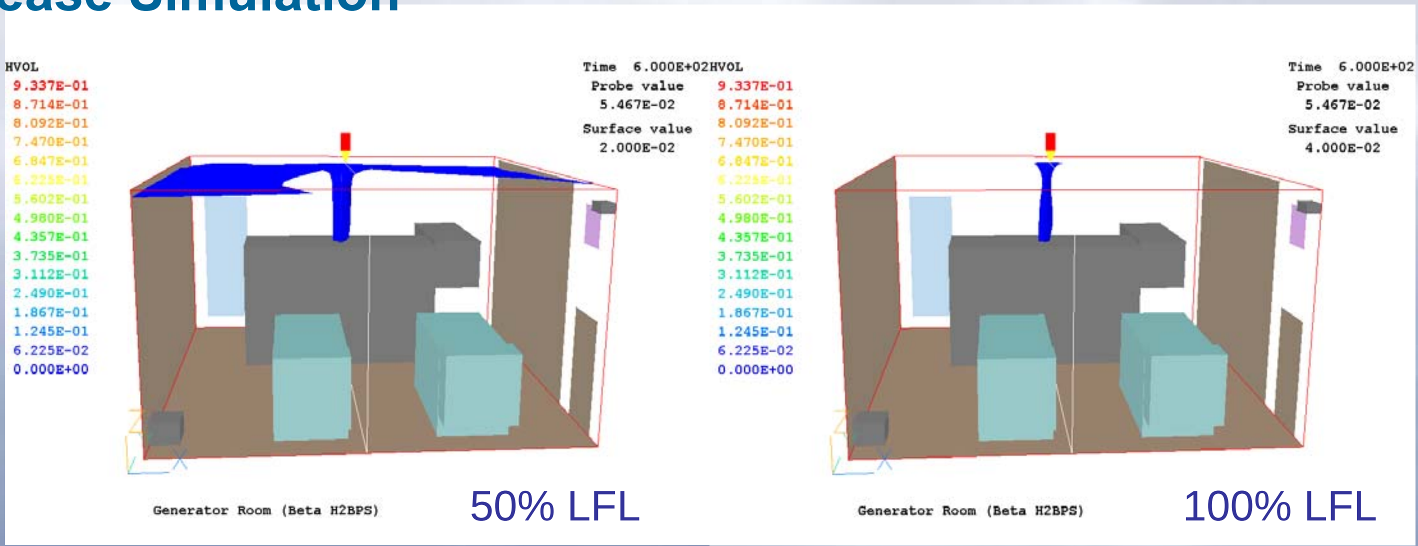
- Existence of louver and exhaust fan in the Generator Room creates a steady-state airflow with 3D fluid flow pattern



Ventilation velocities before release

During-the-Release Simulation

End of 10-min release from the vent line



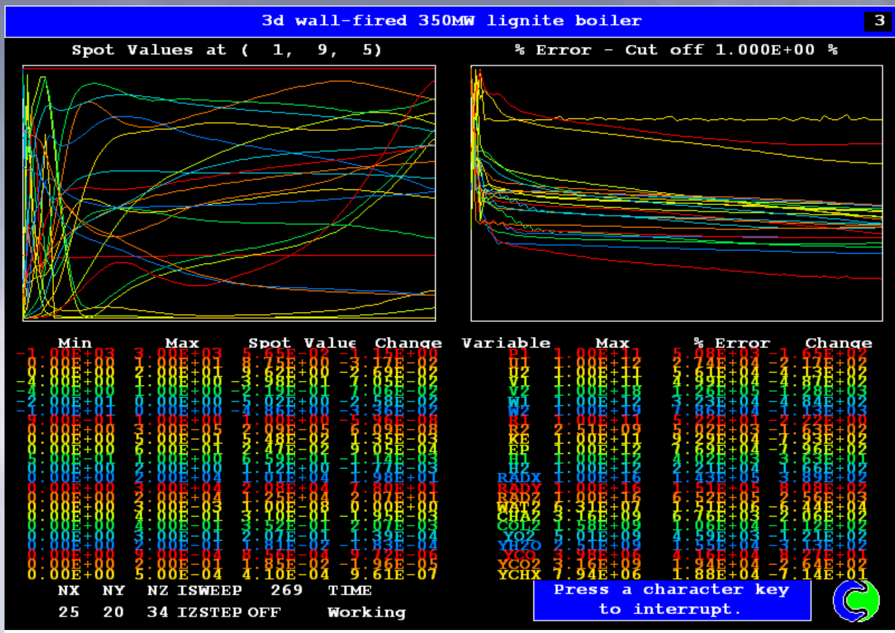
GRAD CFD module: summary

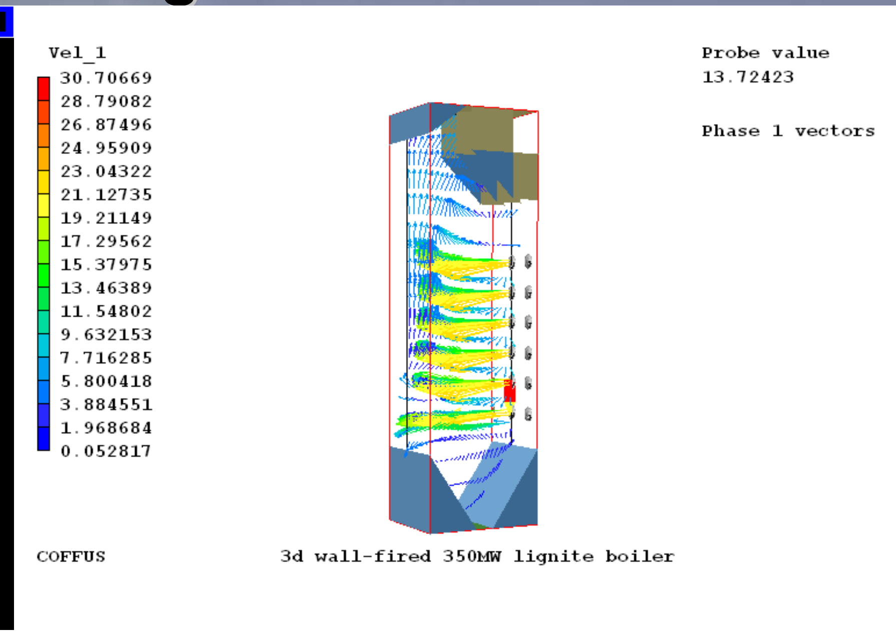
- Advanced GRAD CFD models are developed, validated and applied for various industrial real-life indoor and outdoor releases of flammable gases (hydrogen, methane, propane, etc.)
- Advanced modeling features:
  - Real-life scenarios with complex geometries
  - Dynamic release boundary conditions,
  - Calibrated outlet boundary conditions
  - Advanced turbulence models
  - Real gas law properties applied at high-pressure releases
  - Special output features
  - Adaptive computational grid refinement tools
- Dynamic behaviors of clouds of flammable gas or pollutant could be accurately predicted
- Recommended for safety and environmental protection analyses
- Recommended for design optimizations of combustion devices

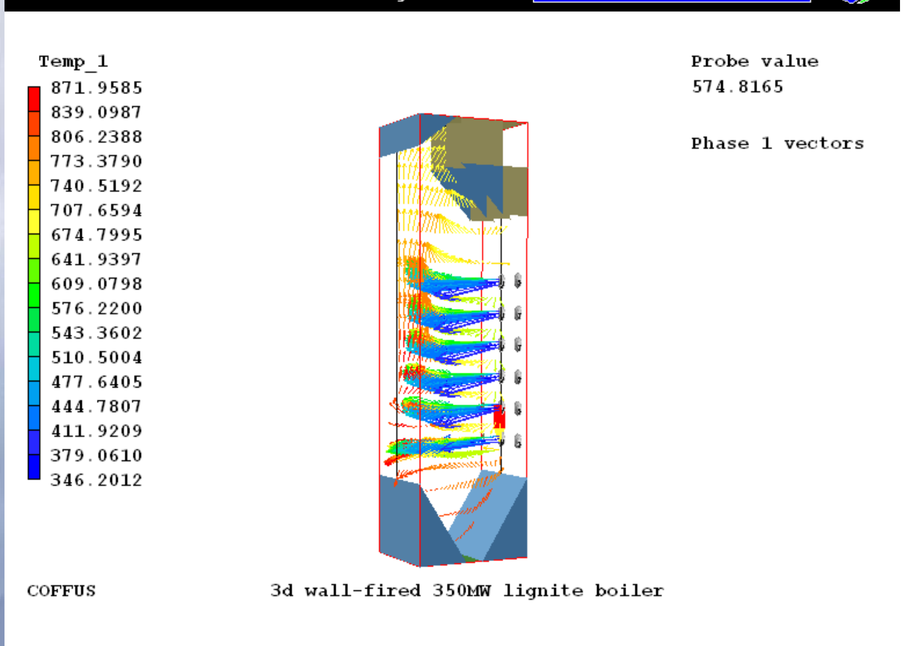
Models of coal gasification and combustion built in PHOENICS (COFFUS, etc.)

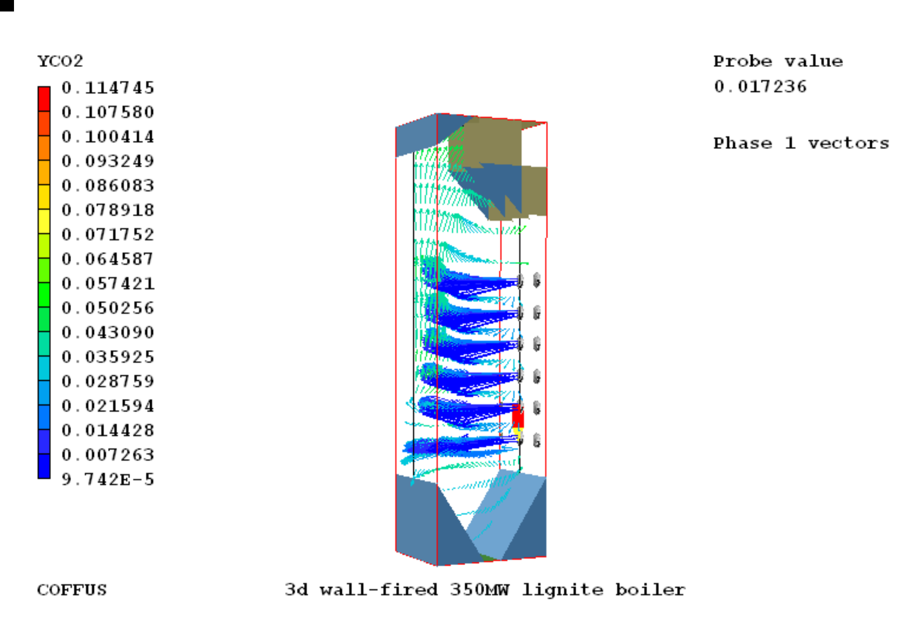
- PHOENICS CFD software has built-in coal gasification and combustion module, COFFUS, capable of modeling coal-fired furnaces (www.cham.co.uk/website/new/mica/coffus.htm)
- COFFUS features:
  - Real-life complex geometries of furnaces
  - Customized inlet boundary conditions (coal composition, coal and gas flow rates, swirl velocities, etc.)
  - Two-phase flow modeling via Eulerian-Eulerian interpenetrating continua with different phase velocities and temperatures and monodispersed approximation (IPSA)
  - Turbulence modeling by k-e model or effective viscosity model
  - Radiation modeling via 6-flux model
  - Devolatilisation and formation of char (solid carbon, ash) modeling by kinetically controlled reaction
  - Char combustion modeling by diffusion controlled heterogeneous reactions (reaction rates inversely proportional to char-particle size)
  - Combustion of volatiles is modeled by EBU model or blended model
  - Output: 3-D distributions of phase velocities, temperatures, species concentrations and radiation fluxes
- Recommended for design optimizations of coal-fired furnaces

COFFUS modeling results









Advanced models of coal gasification and combustion

- List of some models developed for PHOENICS by Dr. Sergei Zhubrin:
- "Combustion in a Moving Coal Bed" (2002): www.cham.co.uk/phoenics/d_polis/d_applic/d_comb/movinbed/movinbed.htm
- "Modelling of Coal Gasification" (2002): www.cham.co.uk/phoenics/d_polis/d_applic/d_comb/coalgas/coalgas.htm
- "Fuel-Dust Flames in a Furnace" (2002): www.simuserve.com/cfd-shop/uslibr/reactive/fur-sing.htm
- "Multi-Fluid Model for Two-step Reaction of Combustion" (2001):
- http://www.simuserve.com/mfm/mfm-cva/two-step/two-step.htm
- "Multi-Fluid Model applied to the combustion of volatiles emerging from solid fuel" (2001): www.simuserve.com/mfm/volatili/volatili.htm
- "Combustion and Nitric Oxide Formation in a Burner" (2001): www.simuserve.com/mfm/mfm-cva/two-step/two-sing.htm
- "Coal-Fired Utility Boiler" (2000): /www.cham.co.uk/phoenics/d_polis/d_lecs/coal/u-boiler/index.htm

Advanced models of coal gasification and combustion - continued

- **Detailed description of coal gasification model:**

  www.cham.co.uk/phoenics/d_polis/d_applic/d_comb/coalgas/coalgas.htm

  Some model features:

  - Non-equilibrium two-phase flow of combustible particles dispersed in carrying air stream is modeled via use of two interpenetrating continua with the transfer of heat, mass and momentum between them
  - Devolatilisation of dispersed phase is kinetically driven
  - Turbulent combustion of volatiles is modeled via two-step reaction of hydrocarbon oxidation, in which carbon monoxide is an intermediate product
  - Char combustion is represented by blended mechanism of oxygen diffusion to the particle and chemical kinetic
  - NOx formation is represented by simplified sub-models, such as oxidation of nitrogen present in the combustion air and that contained in the fuel
  - Turbulence is accounted for by conventional K-e model
  - Radiation is modeled via composite-radiosity model modified to account for radiating particles and gases together
  - Model is applied to pulverized coal combustion in a wall-fired furnace

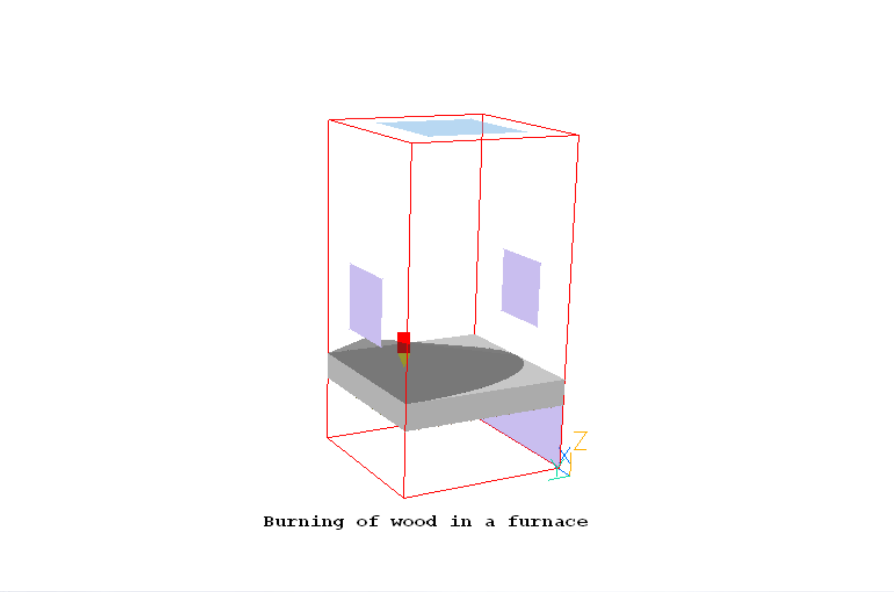
Advanced model of wood/biomass gasification and combustion

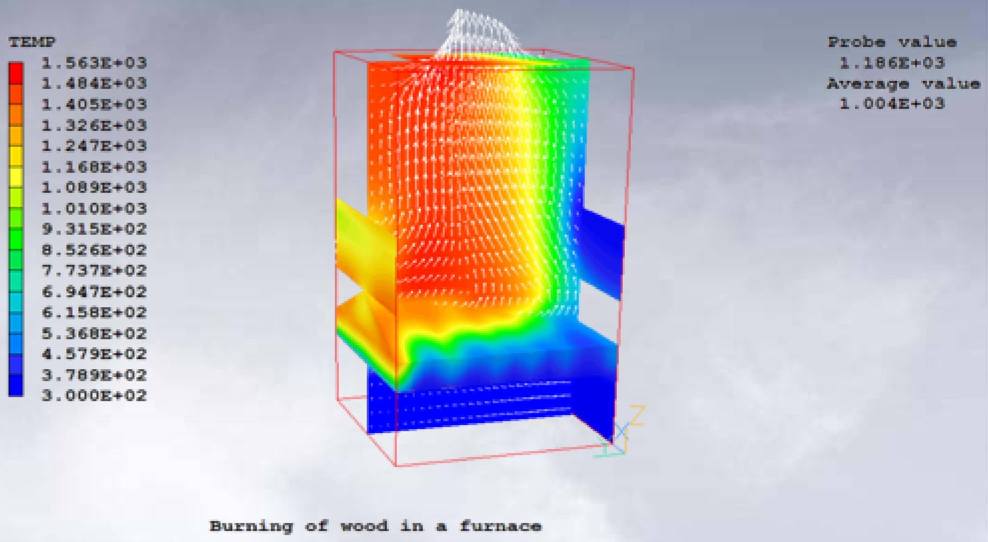
- Some features of model developed by Dr. Sergei Zhubrin:
  - Model of reactive gas flow through the packed bed of wet wooden chips of given composition and size in the real-life over-fed raw-wood-firing furnace of continuous charge type
  - Model uses the Eulerian description of gaseous flow through the porous lump structure with the transfer of heat, mass and momentum between gas and solid phases
  - Fresh lumps of wood are supposed to be fed from over the steady burning bed, which is supported by a grate composed of a number of interlocked bars
  - Primary and over-fire air for combustion enters from outside beneath the grate and through the furnace walls above the bed
  - Gaseous combustion products are discharged through the top opening

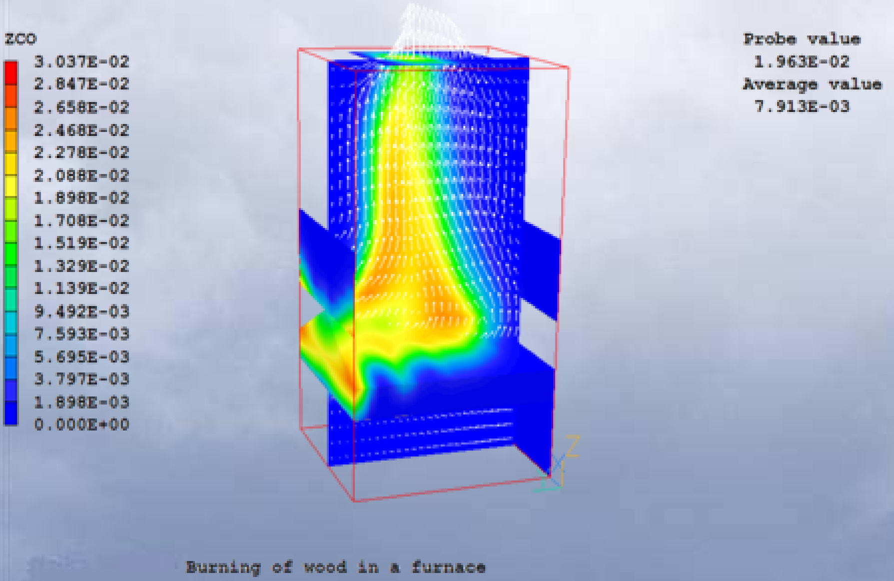
Advanced model of wood/biomass gasification and combustion - continued

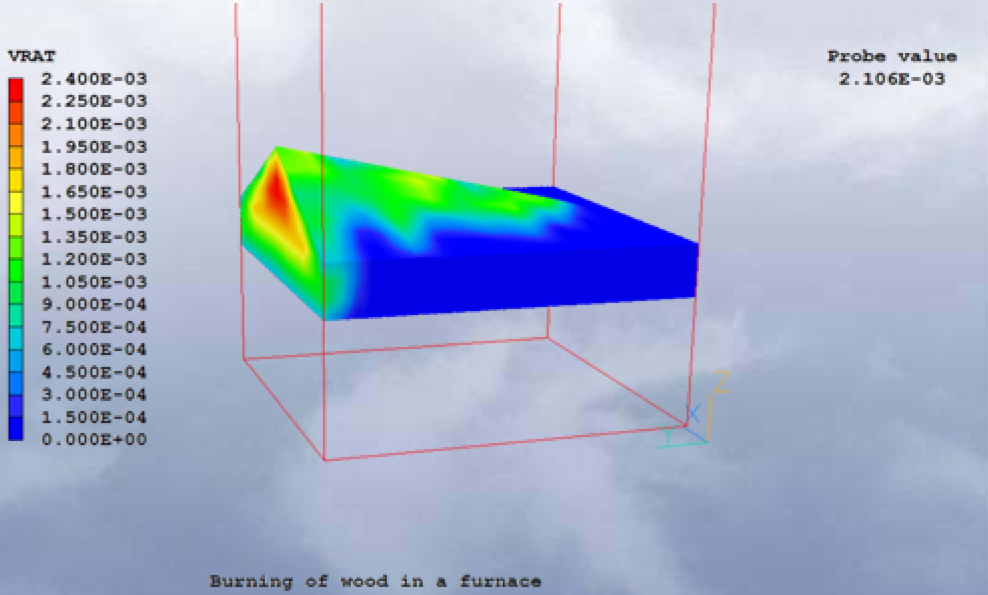
- Some model features (continued):
  - Model predicts the 3-D distributions of velocities, temperatures and product mixture composition in a furnace
  - Model accounts for drying of wet lumps, devolatilisation of wood, char combustion and gaseous combustion
  - Devolatilisation is diffusion-kinetically driven
  - Turbulent combustion of volatiles is modeled via two-step reaction of hydrocarbon oxidation, in which carbon monoxide is an intermediate product
  - Char combustion is represented by blended mechanism of oxygen diffusion to the particle and chemical kinetic
  - Radiation is modeled via composite-radiosity model modified to account for radiating particles and gases together

Advanced model of wood/biomass gasification and combustion - continued









Summary

- **Multiphase CFD research group** at U of T and ACFDA **is capable** of developing, validating and applying the most advanced customized CFD models for various gasification R&D projects
- **Potential applications of expertise:**
  - Development of advanced customized multiphase CFD software modules for real-life industrial applications
  - Model validation
  - Model customization for a particular application
  - Model applications to analyses of complex multiphase flows (gasifier, furnace, separator, pollutant dispersion, safety, etc.)
- **Research team** consists of CFD experts with 25+ years of experience in CFD R&D (both academic and industrial)
- **Products and services**:
  - Advanced customized multiphase CFD software modules for real-life industrial applications (gasification R&D, safety, design)
  - CFD consulting services
  - CFD training and support
- **Approach:**
  - Provide complete set of model development, validation and customization
  - Provide pragmatic and accurate solutions to challenging multiphase problems

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- The authors thank Drs. Andrei Tchouvelev and Zhong Cheng of A.V. Tchouvelev and Associates Inc. for their support and participation in developing GRAD CFD models

Thank you!