Numerical analytical code development at Karlsruhe Institute of Technology KIT
Thomas Jordan, IKET, H2 Group

Technical session 1 – Analytical and experimental research
Fukushima Research Conference – Workshop on Nuclear Hydrogen Safety FRCHS2019
17-18 October, 2019
Outline

- INTRODUCTION
- GASFLOW-MPI
  - Overview
  - Geometry modelling and mesh generation
  - Combustion modelling
  - Film modelling
- COM3D
  - Overview
  - Adaptive Mesh Refinement
  - Fluid-Structure Interaction
- CLOSURE
INTRODUCTION
History of Nuclear Research in Karlsruhe

1956: Reactor Construction and Operating Company mbH Nuclear Research Center Karlsruhe

1995: Research Center Karlsruhe

2009: Karlsruhe Institute for Technology after merger with University

- 1961: Research reactor FR2 44 MW\textsubscript{th}, operation until 1981
- 1965: Multipurpose research reactor MZFR, 58 MW\textsubscript{e}, operation until 1984
- 1971: Compact sodium-cooled nuclear reactor plant Karlsruhe (KNK) 21 MW\textsubscript{e}, operation KNK2 until 1991
- 1971: Reprocessing plant WAK for 35 t/a, operation until 1990

Japanese experts visit the Hydrogen Test Center HYKA
Merger of the University Karlsruhe with the Research Center Karlsruhe in 2009

Research Center Karlsruhe → Campus North
- 15 Programs
- 27 Institutes
- 3,800 Employees
- 305 Mio.€ Budget

University Karlsruhe → Campus South
- 11 Faculties
- 120 Institutes
- 4,000 Employees
- 21,500 Students
- 250 Mio.€ Budget

10 km, 15 min
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Hydrogen Group

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Methods and Tools for Hydrogen Safety
Safety of Flammable Gases, Dusts and Hybrid Mixtures

Theory – Analytical Tools
GASFLOW-MPI
COM3D

Experiments
Hydrogen Test Center

Models – Engineering Correlations
GP-CODE

Models – Engineering Correlations
GP-CODE

Number of methods and tools for hydrogen safety.
State-of-the-Art Containment Safety Code

GASFLOW-MPI
GASFLOW-MPI: “One-Stop-Shopping”
All-speed CFD code for Hydrogen Safety Analysis
Simulate flows at broad Mach number regimes with one all-speed numerical solver

… in the past

All-speed, All physics approach
**GASFLOW-MPI: Features I/III**

- **Flexible geometrical modeling capability**
  - Obstacles
  - Walls and rupture discs
  - Holes
  - Fractional Area/Volume Object Representation (FAVOR)
  - Geometric modeler

- **Flexible structured mesh capability**
  - Cartesian
  - Cylindrical
  - Non-uniform mesh
  - Multi-block
  - Immersed boundary

- **Flexible boundary conditions**
  - Global BC
  - PBC, VBC, MBC, CBC
  - Periodic boundary condition
  - Absorbing boundary condition

- **Proven technology of solving N-S equations and accurate numerics**
  - ICE’d ALE
  - 1st order upwind
  - 2nd order Van Leer
  - Higher order schemes

- **Cutting-edge, scalable and powerful high performance computing capabilities**
  - PETSc
  - Third-party pre-conditioners and solvers
### GASFLOW-MPI: Features II/III

- **Turbulence modelling**
  - Algebraic
  - $\kappa$-$\epsilon$
  - $\kappa$-$\omega$ and SST $\kappa$-$\omega$
  - DES
  - LES

- **Heat and mass transfer, radiation model**
  - Conjugate heat transfer
  - 1-D heat conduction (slab, wall, sink)
  - Radiation model
  - 3-D heat conduction (slab, wall, sink)

- **Multiphase flow**
  - Homogeneous equilibrium model
  - Lagrangian Discrete multiphase model
  - Eulerian multiphase model

- **Combustion models**
  - Eddy break-up
  - Eddy dissipation
  - Arrhenius for detonation
  - Various correlations for turbulent flame velocity

- **Material properties**
  - 25 Gas species
  - 20 solid materials
  - Porous media
### GASFLOW-MPI: Features III/III

#### Unique features for large scale industrial applications

- **Simplified pipe model**
- **Ignitor model**
- **Recombiner model**
- **Sump model**
- **Fan model**
- **Pre-expansion model**
- **Static film model**
- **Spray model based on HEM**
- **Xenon decay model**
- **Sigma and DDT criteria for H2 explosion risk analysis**
- **Aerosol model**
- **Lagrangian dust transportation**
- **Spray model based on Eulerian Multiphase model**
- **Dynamic film model**
- **Dust modeling based on Discrete Multiphase model**
- **Spray model based on Discrete Multiphase model**

#### Pre-processor, Post-processor and data export

- **pyscan**
- **netcdf4**
- **Data format to Third-party post-processing tools**
- **Automatic mesh generation via CAD import**
GASFLOW-MPI: Some Validation References
GASFLOW-MPI: Automatic Mesh Generation
Containment Geometry Modelling

- Large volumes (~100,000 m³)
- Complex multi-connected inside structure
- Mitigation measures

- Use of any standard CAD format IGES, STEP, STL,…
- Selection of spatial resolution
- Automatic wall, obstacle generation and material association, and optimized discretization

Example APR1400:
- 37 individual rooms, including RPV, steam generators and pumps
- Total free volume of ~ 48,000 m³
- Passive Autocatalytic Recombiner equipment
- Ignitor system
- Containment spray system
# GASFLOW-MPI: Validation of combustion models

<table>
<thead>
<tr>
<th>Validation</th>
<th>Facility</th>
<th>Year</th>
<th>Publications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Slow deflagration</td>
<td>THAI HYKA A2</td>
<td>2017</td>
<td>J. Xiao, M. Kuznetsov. <em>NURETH-17</em>, September 3 – 8, 2017</td>
</tr>
<tr>
<td></td>
<td></td>
<td>2017</td>
<td>J. Xiao, M. Kuznetsov.</td>
</tr>
<tr>
<td>Flame acceleration</td>
<td>KIT Detonation tube</td>
<td>2017</td>
<td>J. Xiao, M. Kuznetsov.</td>
</tr>
<tr>
<td>DDT</td>
<td>KIT Ring geometry</td>
<td>2017</td>
<td>J. Xiao, M. Kuznetsov.</td>
</tr>
</tbody>
</table>

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*Images:* Slow deflagration in THAI, Slow deflagration in HYKA A2, Fast deflagration for jet fire in ENACCEF, Detonation in RUT, FA and DDT in ring-shaped geometry.
GASFLOW-MPI: Slow deflagration with heat transfer in THAI-HD44

Turbulent velocity fluctuation \((u')\) at 0 s before ignition

Flame propagation (0 s ~ 15 s)
GASFLOW-MPI: Fast deflagration with heat transfer in ENACCEF

GASFLOW-MPI: Water Film Modelling
Outer Film Model for Passive Containment Cooling System

Example: Passive Containment Cooling System of AP1000
GASFLOW-MPI: Physics of liquid thin film transport

Solid wall: heat conduction

Wall-film interface:
Viscous shear stress, convective heat transfer

Film-gas interface:
Convective heat transfer
Evaporation/boiling
Viscous shear stress

Gas-wall interface:
Convective heat transfer
Steam condensation
Thermal radiation

Gas inside of steel containment

Gas outside of steel containment

Momentum transport at interfaces of gas-film + film-wall

Energy transfer at interfaces of gas-film + film-wall
GASFLOW-MPI: Validation of outer film model with COMMIX Experiments

Film thickness

![Graph showing film thickness vs. location from ellipsoid top](image-url)
Chilton-Colburn empirical analogy

\[ C_f = StPr^{2/3} = St_mSc^{2/3} \quad 0.6 < Pr < 60; \quad 0.6 < Sc < 3000 \]

\[ St_m = \frac{h_d}{u_g} = \frac{Sh}{ReSc} \quad Sc = \frac{\nu}{D_{AB}} \quad Sh = \frac{h_dL}{D_{AB}} \]

\[ h_d = \frac{h_w}{\rho c_p} \frac{Sc^{2/3}}{Pr^{2/3}} \]

and the condensation rate is calculated as:

\[ \dot{m}_s = h_d^* A_w (\rho - \rho_{s, sat}) \]

\[ \rho_{sat} = \frac{P_{sat}}{R_h T_w}, \quad P_{sat} = \exp \left[ \frac{A(T - T_0)}{T + C} \right] \]
GASFLOW-MPI: Non-condensable Gas Absorption in Condensate Film

- The fraction of non-condensable gases in the film $n_{c,film}$:
  \[ n_{c,film} = \frac{P_c}{H_c}, c = O_2 \text{ or } H_2 \]

- The static liquid film:
  - the film on the condense structure are with constant thickness $\delta_{min}$
  - the mass and energy of the film is removed from the control volume when $\int \dot{m}_s dt / A_{film} > \delta_{min}$;
  - Along with the gases dissolved in the film:
    \[ \omega_{c,film} = \omega_{c,g} \frac{P_{gas}}{H_c} \frac{M_{gas}}{M_{film,i}} \]
    \[ \dot{m}_{a,c} = \omega_{c,film} \dot{m}_s \]

Where: $H_c$ is henry constant, $c$ is for components, $H_2$ or $O_2$; $\omega_c$ is the mass fraction, $\dot{m}_{a,c}$ is the absorption rate for component $c$
GASFLOW-MPI: Radiolytic Gas Transport Validation on the Hamaoka Pipe Experiments

Initalional and boundary conditions:
constant p=7MPa, T=286°C
ω_{H_2,g} = 0.002 \ ω_{H_2,g} = 0.016 (mole ration 2:1)
Insulator: calcium silicate wool d=65mm

Mesh: computational domain
2.5 *1.35*7.13m in x, y and z divided 70*8*168 cells
Uniform mesh at pipe cross-section

Test facility for measuring enrichment of non-condensable gases (He/O_2) in the Hamaoka pipe
GASFLOW-MPI: Radiolytic Gas Transport Validation on the Hamaoka Pipe Experiments

Temperature profiles associated with the distance from the upper tube end
GASFLOW-MPI (GF) versus test

Mole fraction at Hp1

<table>
<thead>
<tr>
<th></th>
<th>Test</th>
<th>GF</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hydrogen</td>
<td>64.7%</td>
<td>63.3%</td>
</tr>
<tr>
<td>Oxygen</td>
<td>35.3%</td>
<td>31.7%</td>
</tr>
</tbody>
</table>
GASFLOW-MPI: Applications in Real Scale Containments
Analytical Codes

COM3D
### COM3D: Reactive Flow Modelling

**Since 1995 developed for turbulent combustion in industry relevant scales**

<table>
<thead>
<tr>
<th>Turbulence models</th>
<th>Combustion models</th>
<th>Thermodynamics</th>
</tr>
</thead>
<tbody>
<tr>
<td>Standard k-ε</td>
<td>Integral combustion model KYLCOM</td>
<td>Piecewise linear approximation of JANAF tables</td>
</tr>
<tr>
<td>RNG k-ε</td>
<td>+extensions: quenching, instabilities, DDT, …</td>
<td></td>
</tr>
<tr>
<td>SST k-ε &amp; k-ω</td>
<td>Phenomenological models: EBU, EDC, …</td>
<td>Detonation</td>
</tr>
<tr>
<td>LES Smagorinski,</td>
<td>ALE scheme for slow combustion</td>
<td>Detailed chemistry</td>
</tr>
<tr>
<td>mixed, dynamic</td>
<td>SIMPLE(…) scheme for slow combustion</td>
<td></td>
</tr>
</tbody>
</table>

**Special**

- **Combustible dust model**
- Moving wall boundary conditions (soft wall, fragmentation, …)
- Co-Simulation with ABAQUS

**Cutting-edge, scalable and powerful high performance computing capabilities**

- C++ skeleton with C, FORTRAN routines
- C++ library for domain decomposition
- MPP on basis of MPI (openMPI, …)
- Platforms: Linux clusters; Cray, IBM (SP3, RISC)
- Under development
COM3D: Process Control, Pre-, Post-Processing

- **Meshing**
  - Structured cubic
  - Optimized Load Balancer
  - AMR
  - Immersed 3D Boundaries

- **Pre-Processing**
  - CAD data import
  - comgen
  - Import of GASFLOW data via comcon

- **Post-Processing**
  - GTK+ 3 based GUI
  - VIZIR (incl. on-line mode)
  - Interfaces to all relevant visualization tools

- **Process Control**
  - Client-Server via SUN RPC
  - HDF5 data storage format
COM3D: Typical validation
2 blind large-scale RUT facility simulations

Ignition locations

HYC02
HYC14

Numerical details
- Grid $98 \times 94 \times 416 = 3\,800\,000$ cells
- Cells $6.67 \times 6.67 \times 6.67$ cm
- Process time 0.27 s, 2.4 s
- 80 CPUs with total time ~20000 hours

Initial conditions
- Uniformly mixed $H_2$ / air (11.5% vol.)
- Ignition: channel end, canyon
- $P = 1$ atm, $T = 288$ K

Excellent reproduction of pressure wave evolution in both blind simulations HYC02 and HYC14:
Shown pressure recordings in test HYC02; transducers are located in channel and in upper part of the facility
COM3D: Fluid-Structure-Interaction
Deflagration in flat channel with flexible wall

Wall displacement at $t = 5$ ms determined with COM3D-ABAQUS coupled calculation (co-simulation interface) applying KYLCOM+ combustion model (supported by Toyota Tsusho Europe S.A.)
COM3D: Pipeline deformation and failure behavior under detonation loads

Strain Visualization

Permanent strain experiment vs simulation

Detonation wave experiment vs simulation

Pressure with distance offset x vs Time / s

Permanent strain after test vs Distance / m

"V100G2-Experiment_m.dat"
"V100G2-Model_m.dat"
COM3D: Mitigation of detonation / SW impact

(a) Gas

(b) Dilute two-phase gas-solid medium

(c) Dilute two-phase gas-liquid medium
COM3D: Droplet – flow interaction model

- Disintegration time correlation of Pilch

- Corrected We-number for On > 0.1:

\[
\frac{t_b}{t^*} = \begin{cases} 
6 (\text{We} - 12)^{-0.25} & 12 < \text{We} < 18 \\
2.45 (\text{We} - 12)^{0.25} & 18 < \text{We} < 45 \\
14.1 (\text{We} - 12)^{-0.25} & 45 < \text{We} < 351
\end{cases}
\]

\[
\text{We}_{corr} = \frac{\text{We}}{1 + 1.077 \text{On}^{1.6}}
\]

- Correlation for secondary droplet sizes

\[
\frac{D_{32}}{D_0} = 1.5 \text{On}^{0.2} \text{We}_{corr}^{-0.25}
\]

- Correlation for droplet size distribution

\[
f(D) = \frac{x}{2\sqrt{2\pi} \sigma D} \exp \left\{ -\frac{1}{2} \left[ \frac{x - \mu}{\sigma} \right]^2 \right\}
\]
COM3D: Application Areas

Scientific area: DDT and Detonation using LMR

Industrial area: Automotive, Maritime, H2 Supply, Industry, Nuclear Safety
CLOSURE
User Community and Licensing

GASFLOW-MPI User Community
~ 25 licenses worldwide
(5 Germany, 12 China, 2 South Korea,
2 Mexico, 2 France, 1 Hungary and
1 Czech Republic)
Strong, expanding position in
nuclear community

COM3D User Community
Research focused, universities,
testing of combustion models

License Models
- GASFLOW-MPI: commercial, with services, application focused
- COM3D: research & education; open (free) source
Outlook

GASFLOW-MPI and COM3D
More applications also in the non-nuclear field, e.g. hydrogen supply infrastructure, fuel cells, vehicles, maritime, aviation, space, etc.

GASFLOW-MPI
- Special commercial services, in particular for Asia (spin-off in China)
- Improved user interfaces
- Further acceleration via domain decomposition, GPUs, etc
- Stochastic spray model, porous media, multi-phase H2, particle model,…

COM3D
- Immersed boundaries (moving walls)
- Co-simulation interface
- Shockwave- and flame-water spray interaction