MELCOR Validation against Experiments on Hydrogen Deflagration

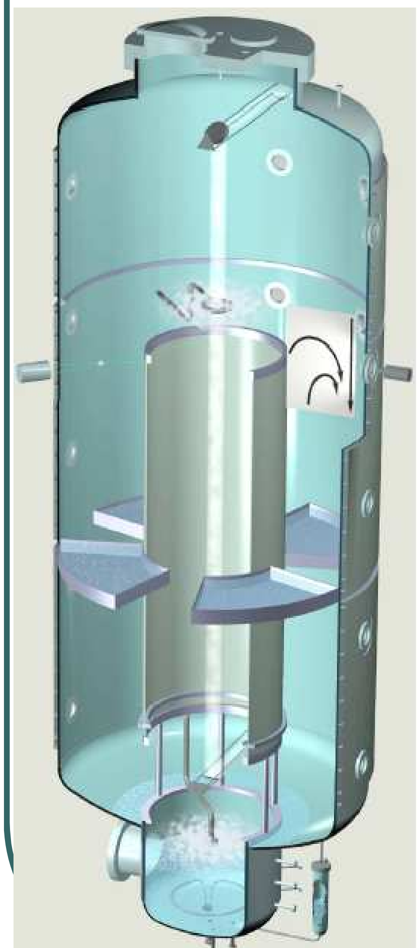
Jiří Duspiva
Nuclear Research Institute Rež, plc.
Nuclear Safety and Reliability Division
Dept. of Severe Accidents and Thermomechanics

3rd European MELCOR User Group Meeting
Bologna, Italy, April 11-12, 2011

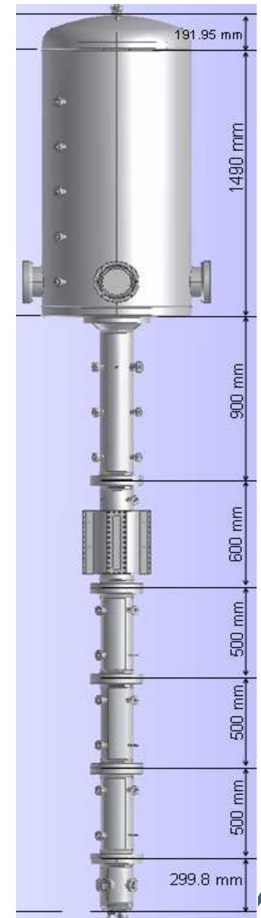
Outline

- ISP-49 MELCOR Application
- Testing of BUR Package
  - Flame propagation
  - Baby case
  - Problems in modeling of deflagration
- Results of THAI HD-2R simulations
- Summary and Conclusions

ISP-49 MELCOR Application
NRI Participation

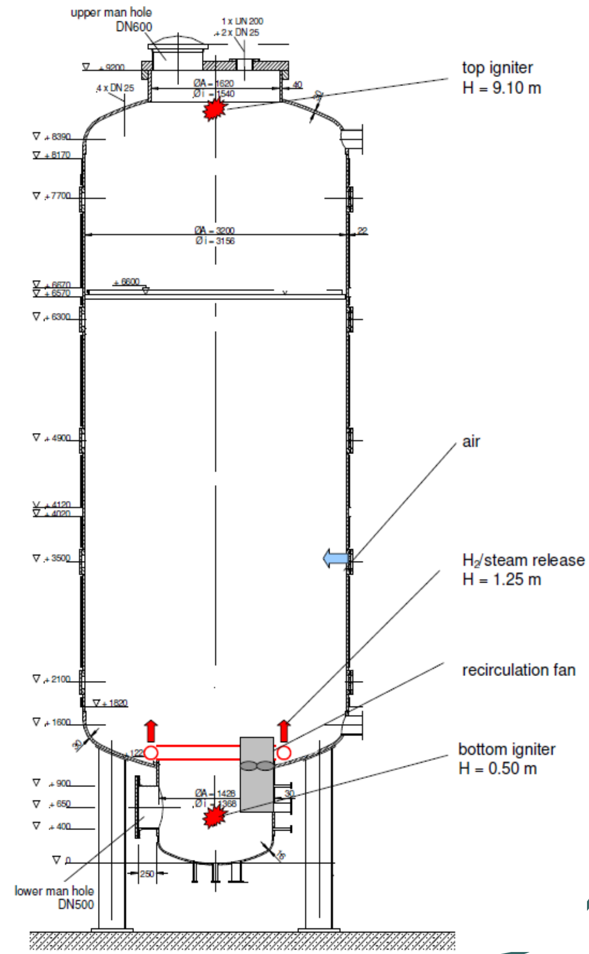


- Main objectives
  - Validation of code against experiments
  - User experience extension to H2 deflagration topic
- ISP-49 – two kinds of experiments
  - THAI Facility – slow deflagration
    - Operated by Becker Technology (Germany)
    - Main interest of NRI (participation in OECD THAI Project)
  - ENACCEF Facility – flame front acceleration
    - Operated by CNRS (France)
    - Minor interest, because MELCOR has no models for Flame Acceleration



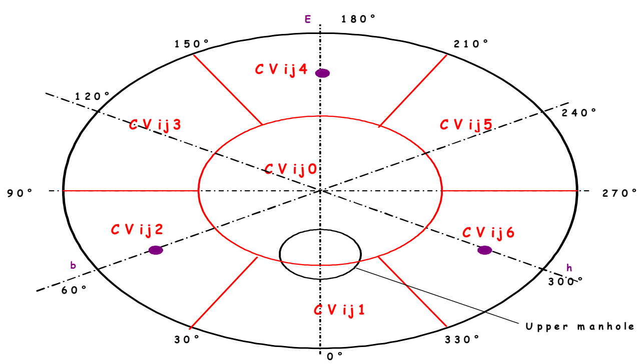
ISP-49 MELCOR Application
Slow Hydrogen Deflagration

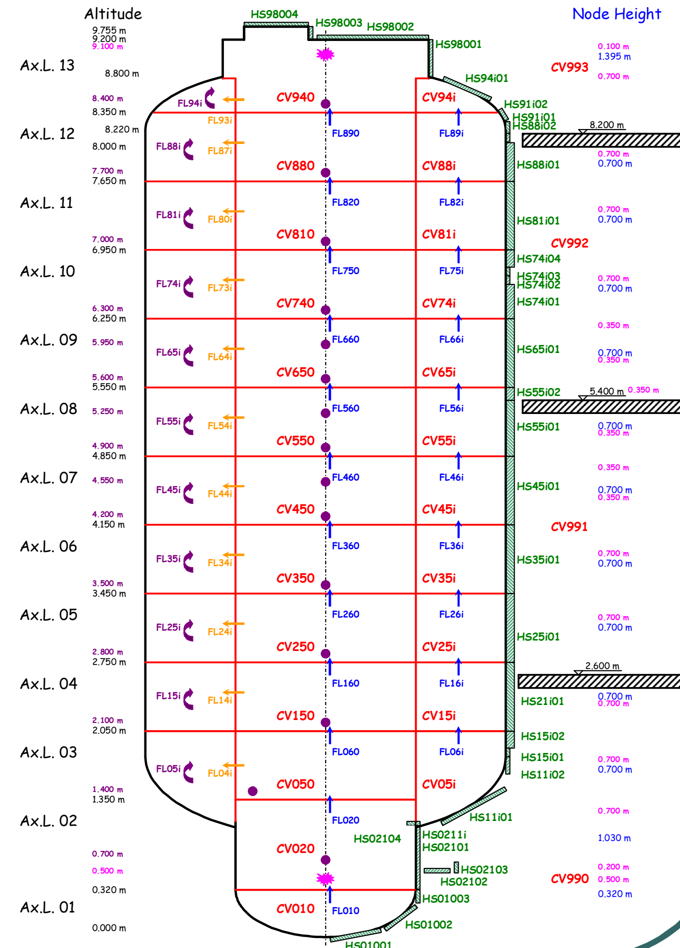
- OECD ISP-49 THAI Tests
  - No internals (only measurement)
  - Deflagration ignited in bottom
  - Homogenized atmosphere
  - HD-2R Test – open calculation
    - H2 concentration 8.0%vol. without steam; temp. 25° C; press. 1.5 bar
  - HD-22 Test – blind and post-blind calc.
    - H2 concentration 10.0%vol. with 25%vol. steam; temp. 90° C; press. 1.5 bar



NRI MELCOR Model
Hydrogen Deflagration Tests

- New input model developed for MELCOR code for OECD-THAI HD test simulation
  - 13 Axial levels, 7 CVs in layer (79+4 CVs, 204 FLs, and 143 HSs)
- Identification of important error in burn propagation among CVs
  - OECD THAI data cannot be shared outside of project members ⇨ Baby Case input model developed for demonstration of error to SNL developers



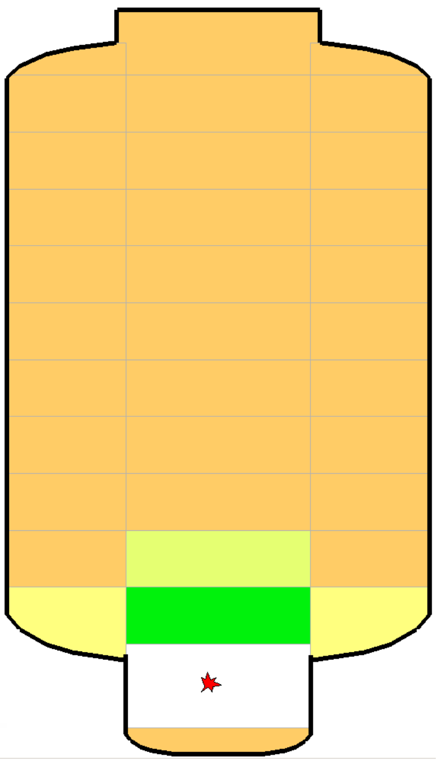


Flame Propagation
Standard MELCOR 1.8.6 YT

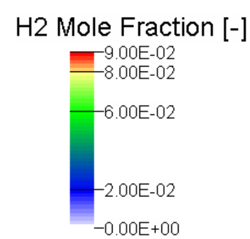
End of burn in bottom CV

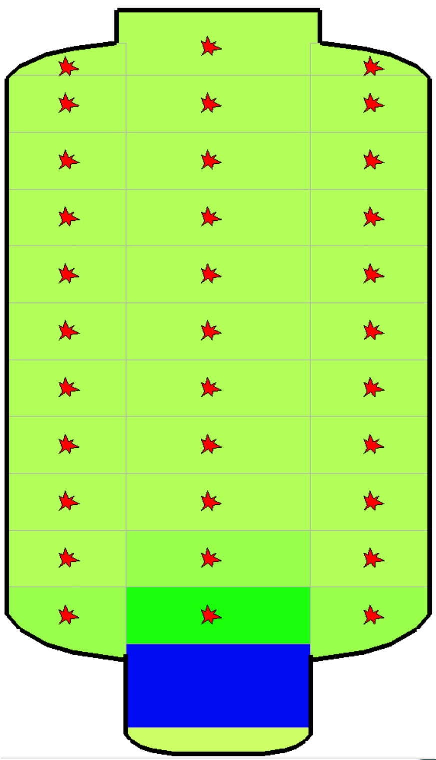
Next time step

Stars indicate instant burns



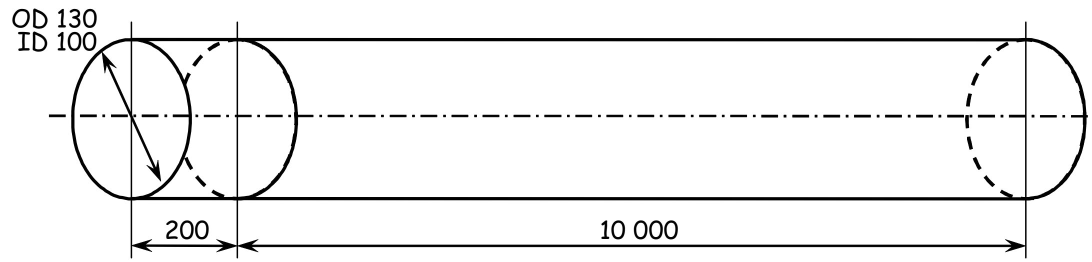
- Identification of important error in burn propagation among CVs
  - OECD THAI data cannot be shared outside of project members ⇨ Baby Case input model developed for demonstration of error to SNL developers

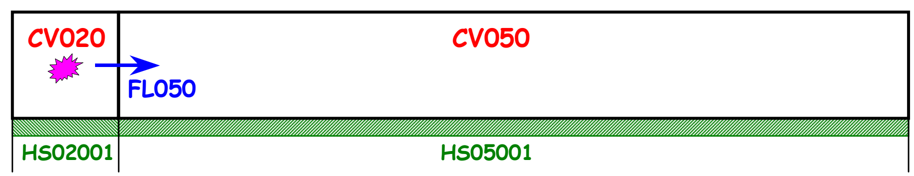


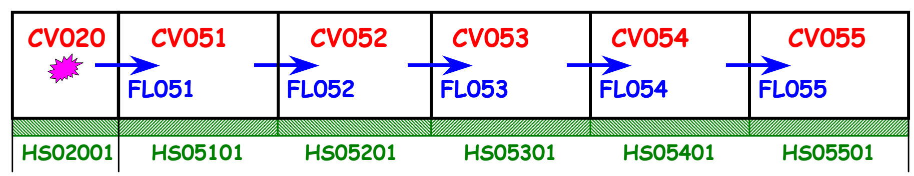


Baby Case
Nodalization Schemes

- Baby case
  - Pipeline with ID 100 mm length 10,200 mm and wall thickness 15 mm
  - First part (200 mm) as space with igniter
- Burning pipe with igniter space
  - End of deflagration should be similar in both models
- 2 CVs model
  - Deflagration propagates from CV020 to CV050
- 6 CVs model
  - Deflagration has to propagate consequently from CV020 to CV051, CV052 …





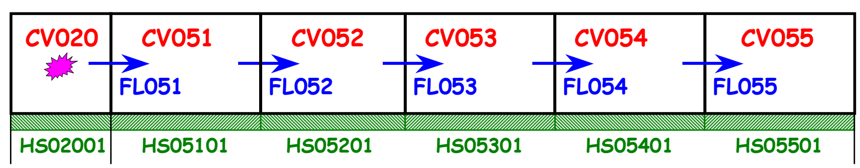


Baby Case Results
Standard MELCOR 1.8.6 YT

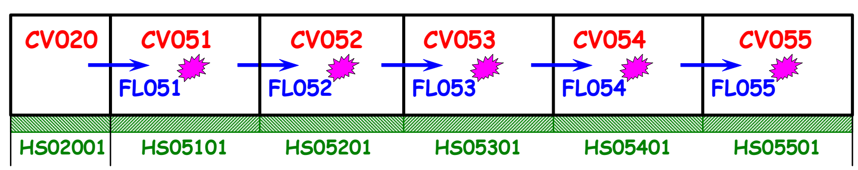
- 2 CVs model
  - Deflagration initiated at t_0 = 0.0 s
  - Propagation from CV020 to CV050 at t_1 = 0.0155 s
  - End of deflagration in CV050 at t_2 = 1.573 s

- 6 CVs model
  - Deflagration initiated at t_0 = 0.0 s
  - But at time t_1 = 0.0155 s deflagration propagated into all remaining CVs simultaneously ⇦ error in propagation algorithm
  - End of deflagration in all CV05i at t_2 = 0.326 s

$0.0\ s < t < t_1$



t_1 = 0.0155 s

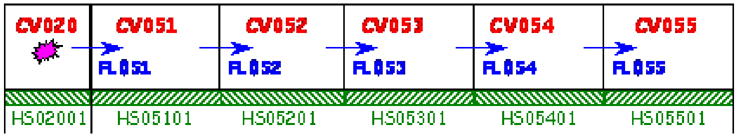


Baby Case Results
Improvement of MELCOR 1.8.6

- NRI debugging of this error resulted in identification of correction needs in two routines (burprp.f and burrun.f)
  - Deflagration initiated at t_0 = 0.0 s End time in 2CVs model t_2 = 1.573 s

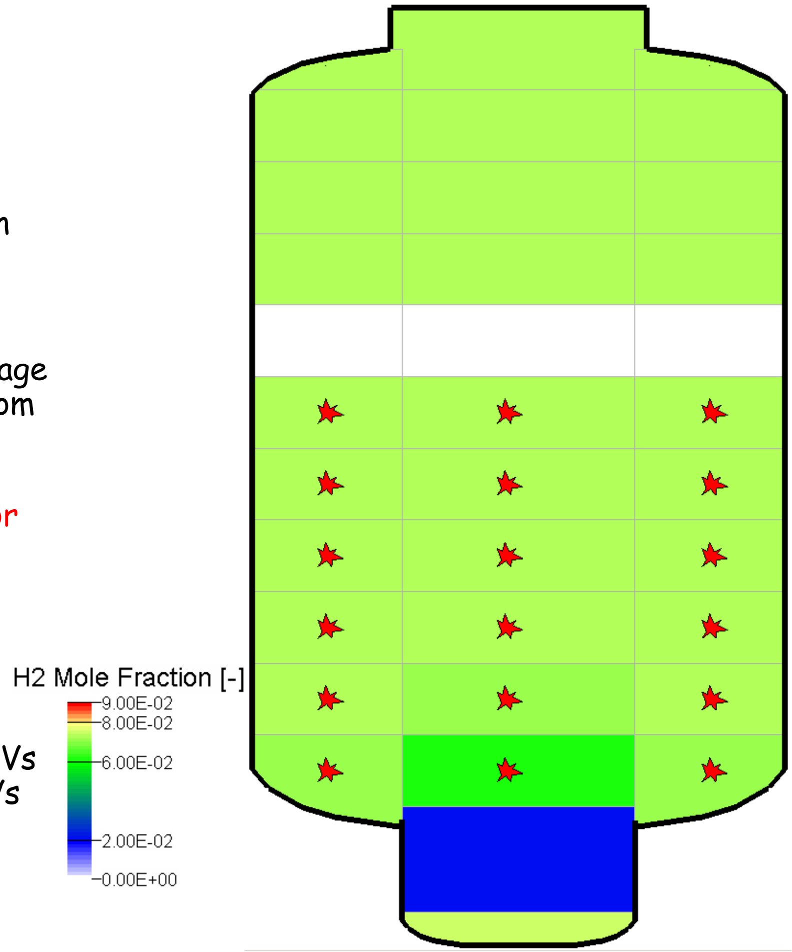
Standard M186		Improved M186	
Propagation into CV051	1.59547E-02 s	Propagation into CV051	1.59547E-02 s
Propagation into CV052	1.59547E-02 s	Propagation into CV052	3.41714E-01 s
Propagation into CV053	1.59547E-02 s	Propagation into CV053	7.11714E-01 s
Propagation into CV054	1.59547E-02 s	Propagation into CV054	1.06171E+00 s
Propagation into CV055	1.59547E-02 s	Propagation into CV055	1.40171E+00 s
End in CV055	3.36495E-01 s	End in CV055	1.73171E+00 s

- Observations and modifications reported to SNL developers including Baby Case inputs (BUG Report 287)
  - Added refilling of burning tube with hydrogen and oxygen and initiation of subsequent deflagration ⇨ second set of deflagrations again propagated into all CVs simultaneously, one more routine modified (burcom.f) to correct subsequent deflagrations



Flame Propagation
Standard MELCOR

- NRI performed set of other tests
  - Testing of older version (MELCOR1.8.5) against baby case with additional source of hydrogen (SNL modification)
    - MELGEN failed due to incompleteness of hydrogen source definition
    - MELGEN YT_1010 and YU_2798 do not check existence of appropriate external energy source related to external mass source as described on page CVH-UG-26 (full description in BUG339 report from end of February 2009)
    - MELCOR 1.8.6 (and also 2.1) corrected to fulfill request on existence of external energy source for each of external mass source
    - It is solved in subversion 3037 of M186 and 1191 of M2.1
  - Additional testing of propagation with standard release of MELCOR 1.8.6 YT_1010
    - Zero hydrogen concentration in one (or more) of CVs on propagation chain of CVs preserve remaining CVs from immediate deflagration propagation
      - Important for older Cntn analyses

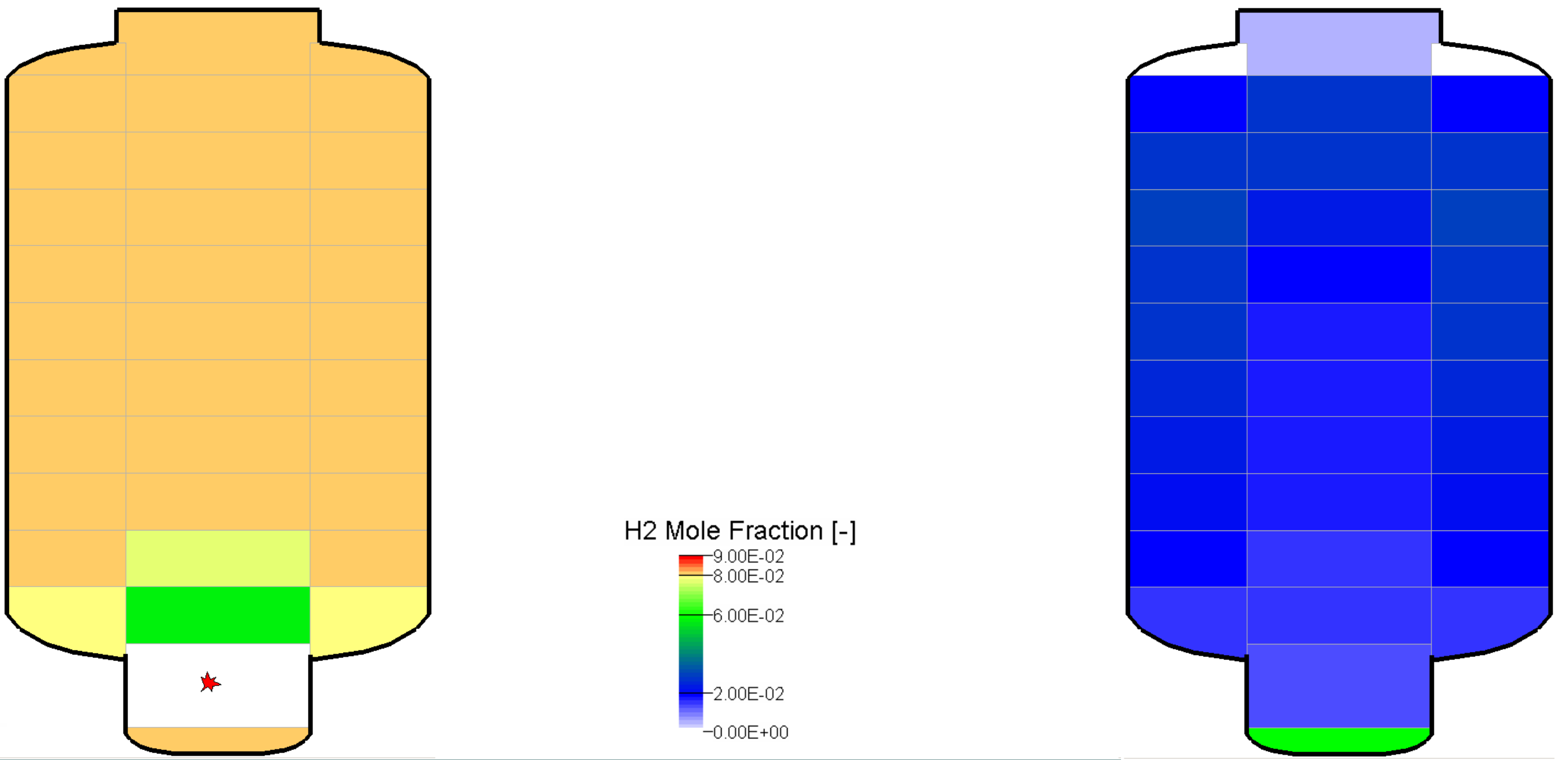


Flame Propagation
Improved MELCOR 1.8.6

End of burn in bottom CV

Next time steps

Stars indicate instant burns



Modeling of Deflagration
Problematic Topics

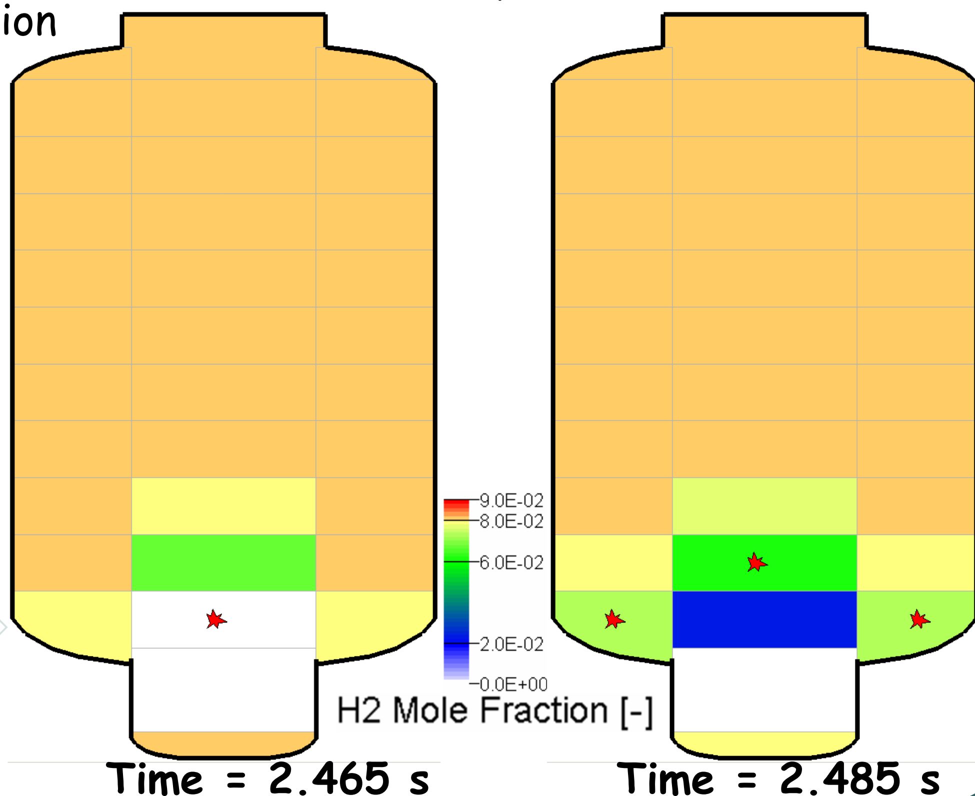
- Some problematic topics identified in MELCOR application to THAI HD-2R test
  - Significantly faster flame propagation
    - Flame speed determination
  - Remaining unburnt hydrogen
    - Effect of lumped parameter approach to combustion completeness
  - Rate of hydrogen consumed from burning

Modeling of Deflagration
Flame Speed Determination

- MELCOR uses only one correlation for all flame directions (upward, downward, and horizontal)
- NRI prepared updated definition of SC2200 for application within ISP-49
  - Based on OECD THAI HD tests
    - Proprietary source
  - Relevant only for upward flame propagation
    - It cannot be recommended for plant simulations
  - It played important role in HD-22 test simulation, where under-predicted flame velocity resulted in absence of deflagration in central nodes of upper half of vessel
    - Corrected with realistic flame velocity ⇦ impact of ATM overflow

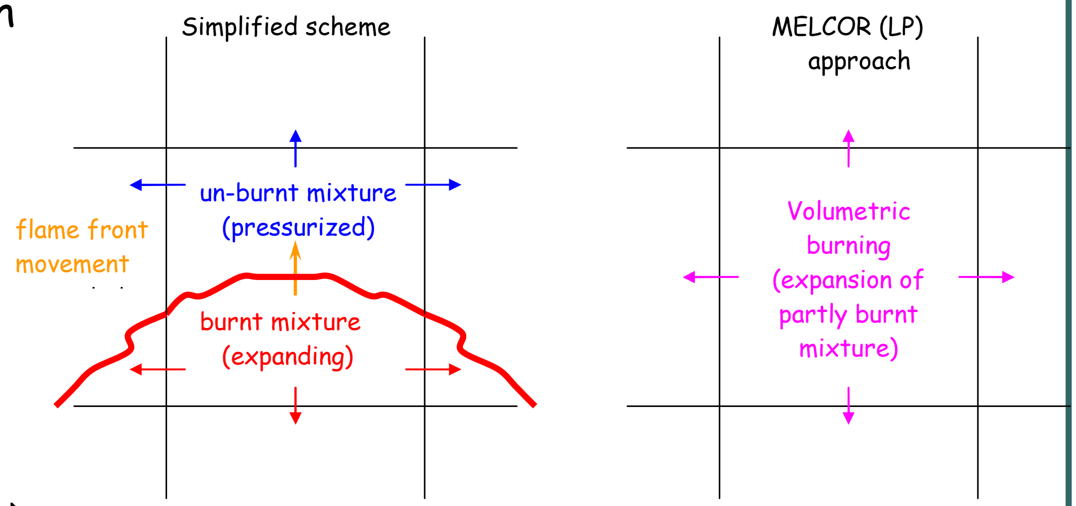
Modeling of Deflagration
Lumped Parameter Approach (1)

- Full combustion completeness is defined ⇨ H2 mole fraction is 0.0 at the end of deflagration in lower CV
- Continuation of deflagration in adjacent CV results in ATM pressurization in recently burning CV and its expansion ⇨ overflow into all adjacent CVs
- MELCOR code does not distinguish atmosphere composition in front and behind flame front position – ATM is fully homogeneous
- Due to instant combustion, ATM flowing into other CVs is
  - H2 lean in comparison with CV in front of flame front propagation (here above) ⇨ decrease of H2 mole fraction
  - H2 rich in comparison with CV behind flame front (here below) ⇨ increase of H2 content, which remains unburnt



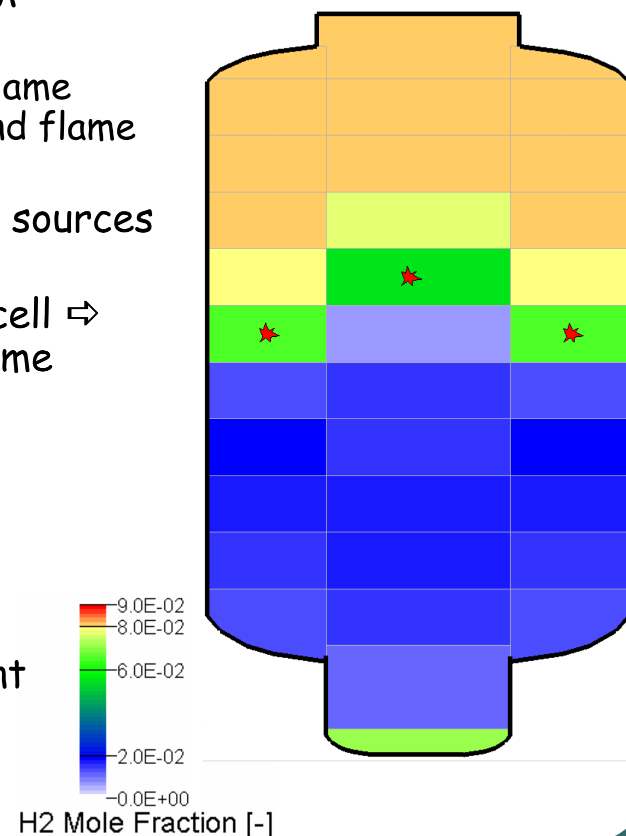
Modeling of Deflagration
Lumped Parameter Approach (2)

- Full combustion completeness is defined ⇨ H2 mole fraction is 0.0 at the end of deflagration in lower CV
- Continuation of deflagration in adjacent CV results in ATM pressurization in recently burning CV and its expansion
  ⇨ overflow into all adjacent CVs
- MELCOR code does not distinguish atmosphere composition in front and behind flame front position – ATM is fully homogeneous
- Due to instant combustion, ATM flowing into other CVs is
  - H2 lean in comparison with CV in front of flame front propagation (here above) ⇨ decrease of H2 mole fraction
  - H2 rich in comparison with CV behind flame front (here below) ⇨ increase of H2 content, which remains unburnt



Modeling of Deflagration
Lumped Parameter Approach (3)

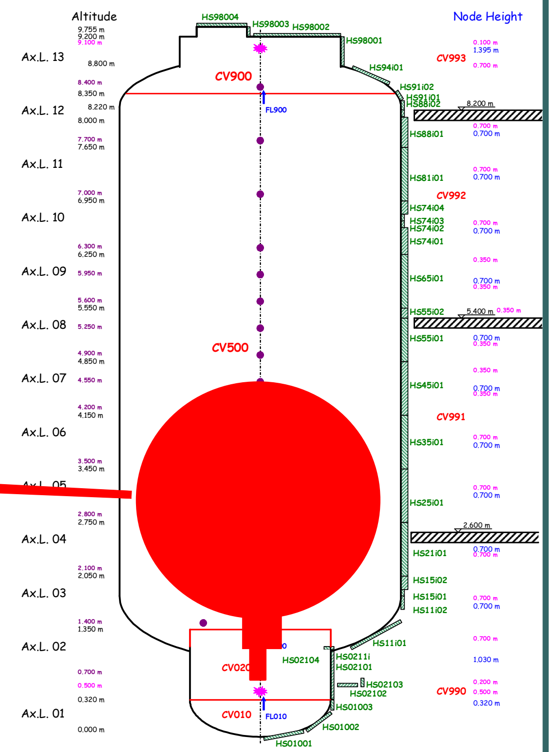
- Is it possible to find any user solution?
  - MELCOR has no capability to filter one or more ATM components in flow paths ⇨ **No**
    - More over MELCOR does not know orientation of flame movement and position of sides – in front and behind flame front (volumetric combustion approach)
  - MELCOR has capability of external mass and energy sources and sinks ⇨ **Possible user solution**
  - MELCOR has capability to define igniter in each of cell ⇨ **Possible user solution** (necessary modification of some model parameters - XH2IGY, XH2CC, and XH2PDN)
- Is complicated nodalization best approach for MELCOR?
  - More variants of nodalization prepared and tested
  - Some models had also subversions
  - Results processing focused on – timing of flame front position, pressure evolution, and unburnt mass of hydrogen

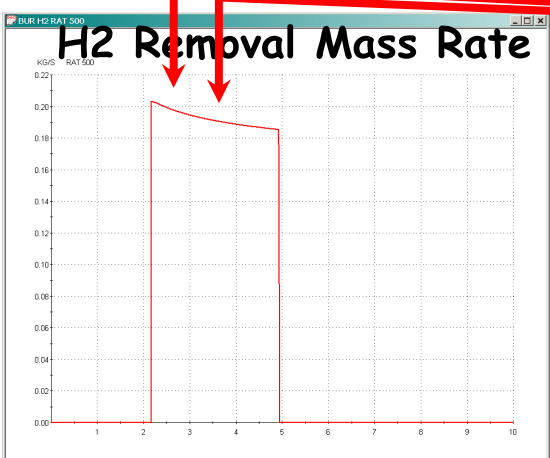


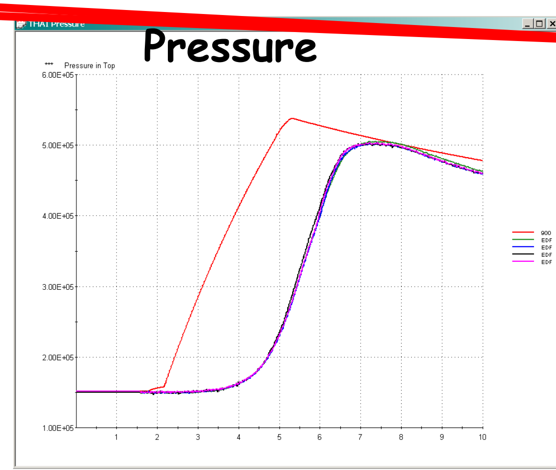
Modeling of Deflagration
Hydrogen Removal Rate

- Duration of deflagration is calculated from characteristic dimension (of control volume) and flame speed
- Flame speed is calculated from concentrations at beginning of burn, but
- Rate of hydrogen consumed from burning is calculated from current concentrations in each time step and it is proceeded in whole volume
  - Real burn is proportional to surface of flame front (spherical shape)
- Deflagration is terminated after predicted duration (point 1)
- Those effects occurred in all CVs and in all input models, but in this case is very well visible

4CVs Model





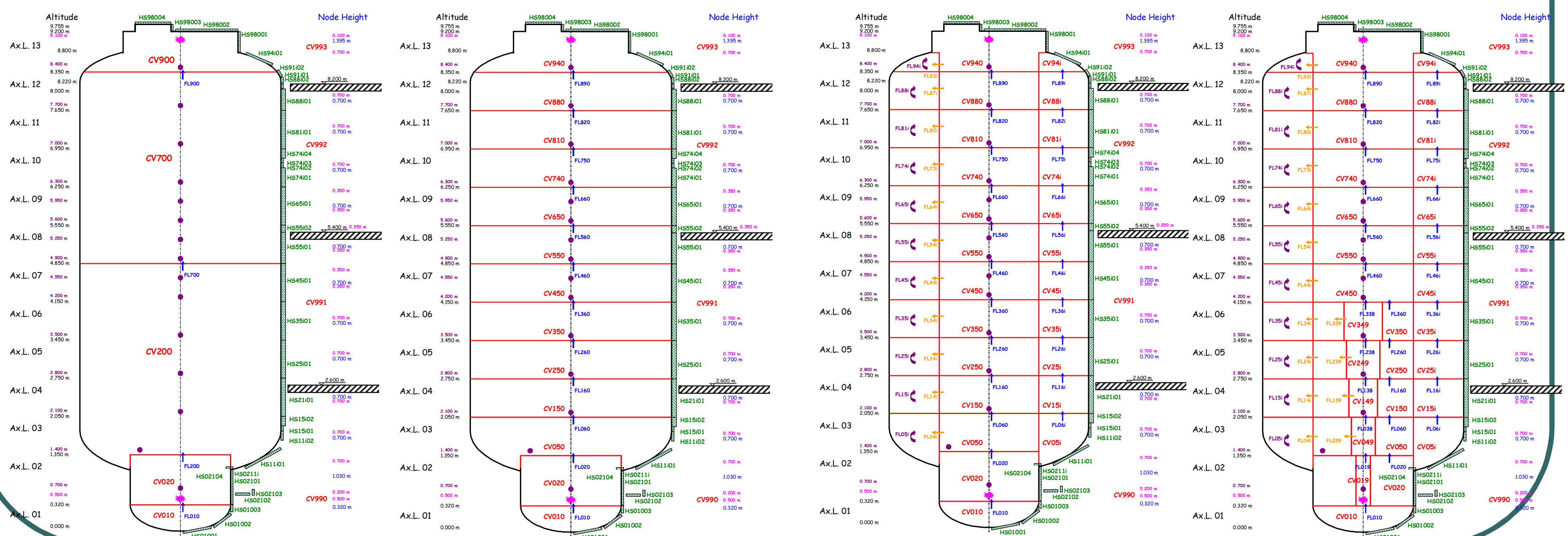


Simulation of HD-2R Test
Impact of Nodalization

- 5 nodalizations prepared
- Specific user approaches defined
  - S&S – H_2 sinks defined behind flame front and appropriate sources in front of it
  - Ign - igniters in CV behind flame front

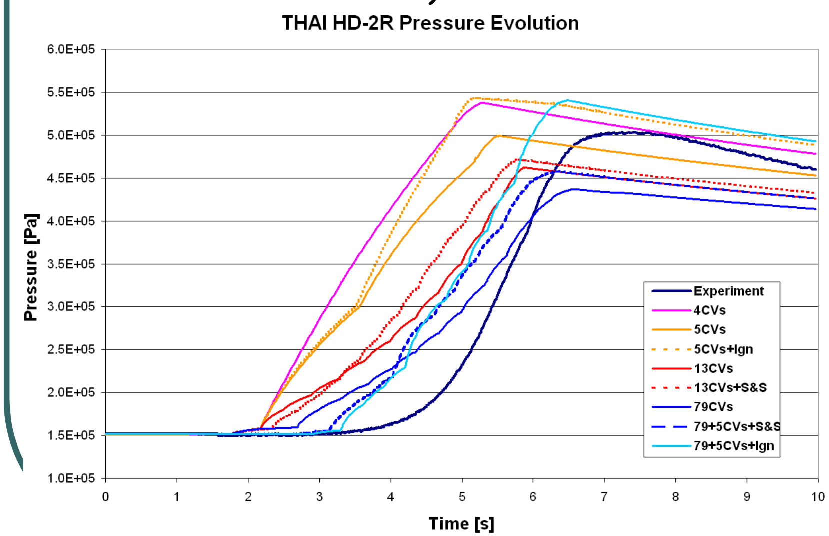
4CVs **13CVs** **79+5CVs+S&S**

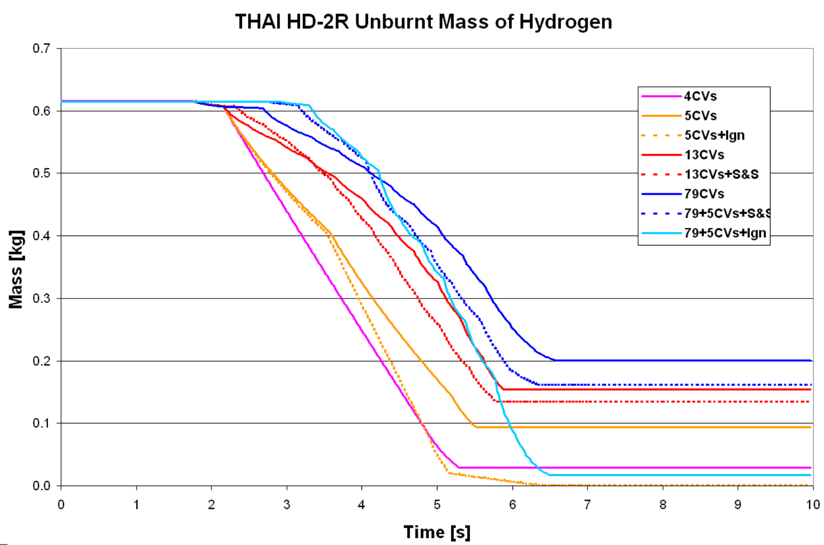
5CVs 5CVs+Ign **13CVs+S&S** **79CVs** **79+5CVs+Ign**



Simulation of HD-2R Test
Impact of Nodalization (2)

- Best agreement between simulation and measured pressure history
  - Maximum pressure 5CVs
  - The simplest case **4CVs** (usual approach to Cntn) slightly overestimated pressure maximum and significantly earlier onset of pressure increase – immediate deflagration in big volume
  - Cases with additional igniters 5CVs+Ign and 79+5CVs+Ign slightly overestimated pressure maximum, but they predict correctly combustion completness
    - Probably due to underestimation of heat losses from flame front to walls (absence of radiation)





Summary and Conclusions

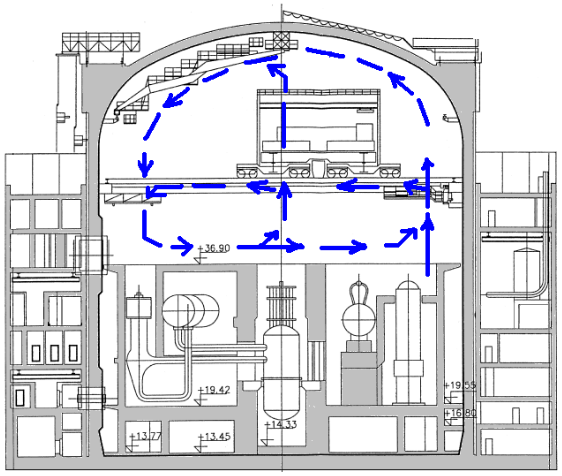
- Validation of MELCOR code against deflagration tests resulted in
  - Code correction – flame propagation algorithm
  - Observations concerning problems with more detail nodalizations
    - LP approach effect – redistribution of H2 to already burnt CVs
    - Flame speed prediction using default correlation
    - Rate of hydrogen removal during deflagration
    - Code has no modeling capability for flame acceleration
  - It is not possible to suppose any improvement without important and principal changes of source code and BUR package model, but
  - Code is flexible
    - It allows to define more realistic flame speed profile via. CF (if it is known)
    - It allows to use some user approaches (if user knows results)

Summary and Conclusions (2)

- Generally H_2 deflagration is important, but deflagration itself is very fast process and its very detail modeling within whole plant simulation seems not be necessary
  - But LP effect could influence prediction of H_2 distribution in detail Cntn nodalizations, if any deflagration is predicted
- Integral application of MELCOR code to source term estimation in scenario with hydrogen deflagration is possible
  - Duration of deflagration is very short in comparison with whole scenario
  - Whole plant input models include usually coarse nodalization (more rooms are merged into one CV or one CV per room) – case 4CVs showed relatively good agreement in maximum pressure
- H_2 distribution requests very detailed nodalization, but it results in absolutely wrong prediction of deflagration
  - Study on impact of nodalization is needed
- MELCOR is not suitable code for detailed study of H_2 combustion

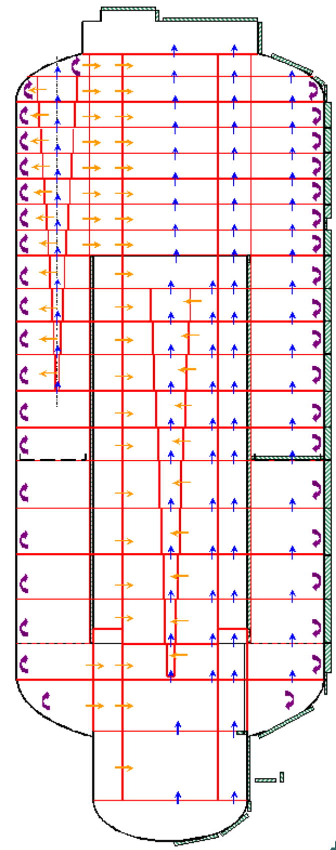
Conclusions on Cntn Modelling (1)

- User has to anticipate convection loops in containment, mainly in large open space (reactor hall) and to develop nodalization with taking of such loops into account
  - Only one CV for reactor hall can't simulate any circulation
- Recommendation on FL definition between virtually subdivided big space
  - Prepared by Dr. Sonnenkalb (GRS) based on comparison of MELCOR to COCOSYS
    - Presentation at the 1st EMUG Meeting 12/2008
    - FLARA reduced to max 20 m2, FLLEN max 10 m
    - In my THAI model I used real values of FLARA, FLLEN, SAREA, and SLEN, but in Cntn I used reduced values for SLEN (0.1 m)

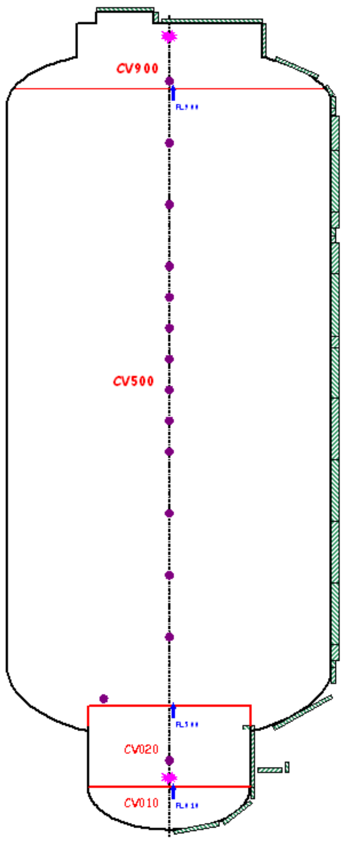


Conclusions on Cntn Modelling (2)

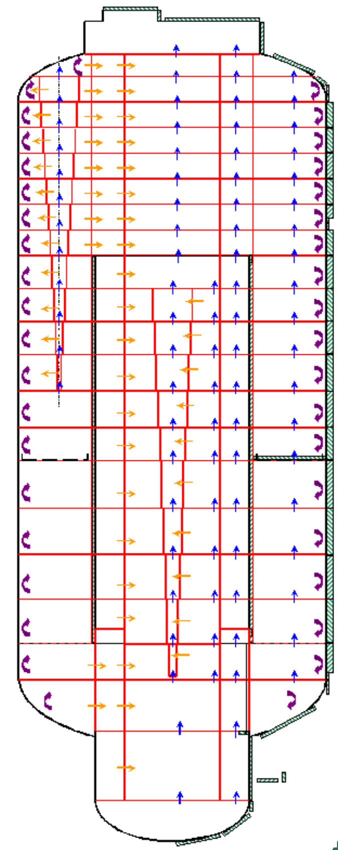
- OECD THAI Project – Benchmark on HM2 test
  - Recommendation to model CVs and FLs of upward directed plumes
    - Flow is directed with pressure difference, which depends on hydrostatic head and it is function of atmosphere density
    - If light gas enters to big volume, it is immediately homogenized with content of this CV, but
    - If upward plume is simulated with independent set of CVs, pressure difference is kept and buoyant force is predicted correctly
    - Problematic topic – angle depends on plume and ATM composition, but
      - They vary during plant simulations, but nodalization is fixed



Conclusions on Cntn Modelling (3)



- H2 distribution requests very detailed nodalization, but it results in absolutely wrong prediction of deflagration and vice versa – coarse nodalization predicts relatively good response of deflagration, but absolutely wrong H2 distribution
- Testing of MELCOR on THAI HR tests with detailed nodalization confirmed correct modelling (data are proprietary)
    - MELCOR can be used for Cntn simulation with robust hydrogen removal system based on PAR with very detailed Cntn nodalization
        - Robust means – no hydrogen deflagration
- Plant simulations on H2 distribution and hydrogen removal system with stand alone Cntn
    - Elimination of primary system prediction feedback
    - Study on separation performed with MELCOR 1.8.5
        - Contribution to MCAP 2005
        - Should be repeated with M186 (and M2.1 ?), then presented (next EMUG?)



End of Presentation

Thank You for Your Attention