Compilation of Spray A Modeling Efforts

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Sibendu Som
Argonne National Laboratory

Engine Combustion Network (ECN) Workshop 2011

Participants

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Presentation Schedule

4:15pm: Spray A Computational Efforts (Introduction): Sibendu Som, Argonne

4:20pm: Modeling approaches by different groups

Argonne: Sibendu Som
UW-Madison: Chris Rutland
ICE-Polimi: Gianluca D'Errico
Sandia: Lyle Pickett
UNSW: Yuanjiang Pei

5:10pm: Spray A Computational Results Comparison: Sibendu Som, Argonne

5:40 – 6:10pm: Discussion

Outline

- ❑ Baseline Spray A: non-reacting conditions
- ❑ Spray penetration vs. time
  - ✓ Effect of grid size
  - ✓ Effect of time-step size
  - ✓ Effect of turbulence model
- ❑ Vapor penetration vs. time
  - ✓ Effect of grid size
  - ✓ Effect of time step size
  - ✓ Effect of turbulence model
- ❑ Mixture fraction at different radial positions
  - ✓ Two axial positions were chosen for comparison
- ❑ Comparison of vapor boundary location
- ❑ Comparison of liquid boundary location
- ❑ 2 optional test cases investigated
  - ✓ Similar grid sizes, models, model constants identified
  - ✓ No comparison against experimental data
- ❑ Discussion & Future work!

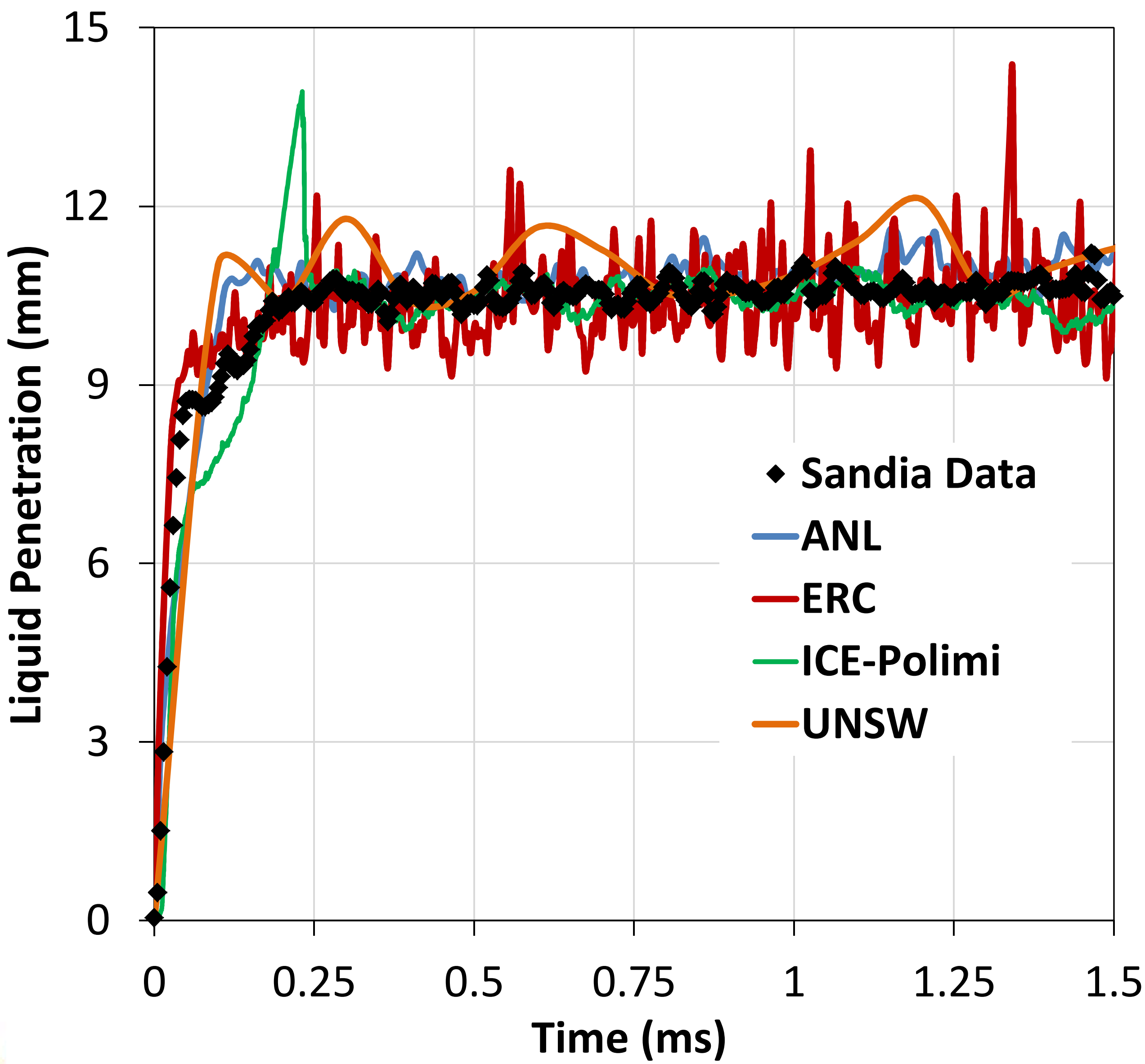
Baseline Spray A: non-reacting conditions

Parameter	Quantity
Fuel	N-dodecane (n-$C_{12}H_{26}$)
Nozzle outlet diameter	90 μm
Nozzle K-factor	1.5
Nozzle shaping	Hydro-eroded
Discharge coefficient	0.86
Fuel injection pressure	150 MPa
Fuel injection temperature	363 K
Injection duration	1.5 ms
Injected fuel mass	3.5 mg
Injection rate shape	Square
Ambient gas temperature	900 K
Ambient gas pressure	6.0 MPa (approx.)
Ambient gas density	22.8 Kg/m^3
Ambient Oxygen Concentration	0 %

Quick Recap

	ANL	ERC	ICE-Polimi	UNSW
Code/Software	CONVERGE	KIVA-ERC	OpenFOAM	FLUENT
Turbulence models	Standard k-ε, RNG k-ε, LES- Smagorinsky	Dynamic structure LES	Standard k-ε, RNG k-ε, Realizable k-ε	Realizable k-ε
Spray models: Injection Atomization & Breakup Collision Drag Evaporation	Blob KH-RT NTC Dynamic Frossling	Blob KH-RT O'Rourke Aerodynamic Frossling	Huh-Gosman Bianchi, Wave No Dynamic Frossling	Blob Wave O'Rourke Stokes-Cunningham Frossling
Grid: Type Dimensionality Smallest grid size	Structured with AMR Full-3D domain 0.125 mm-LES, 0.5 mm-RANS	Structured Cartesian 3D-Axisymmetric 0. 50 mm - LES	Structured with ALMR Quarter-3D domain 0.5 mm	Structured 2D-Axisymmetric 0.25 mm
Time discretization	PISO	KIVA-SIMPLE	PISO, SIMPLE	PISO
Preferred time-step size (ms)	Variable	Variable	5.0E-7	1.0E-7

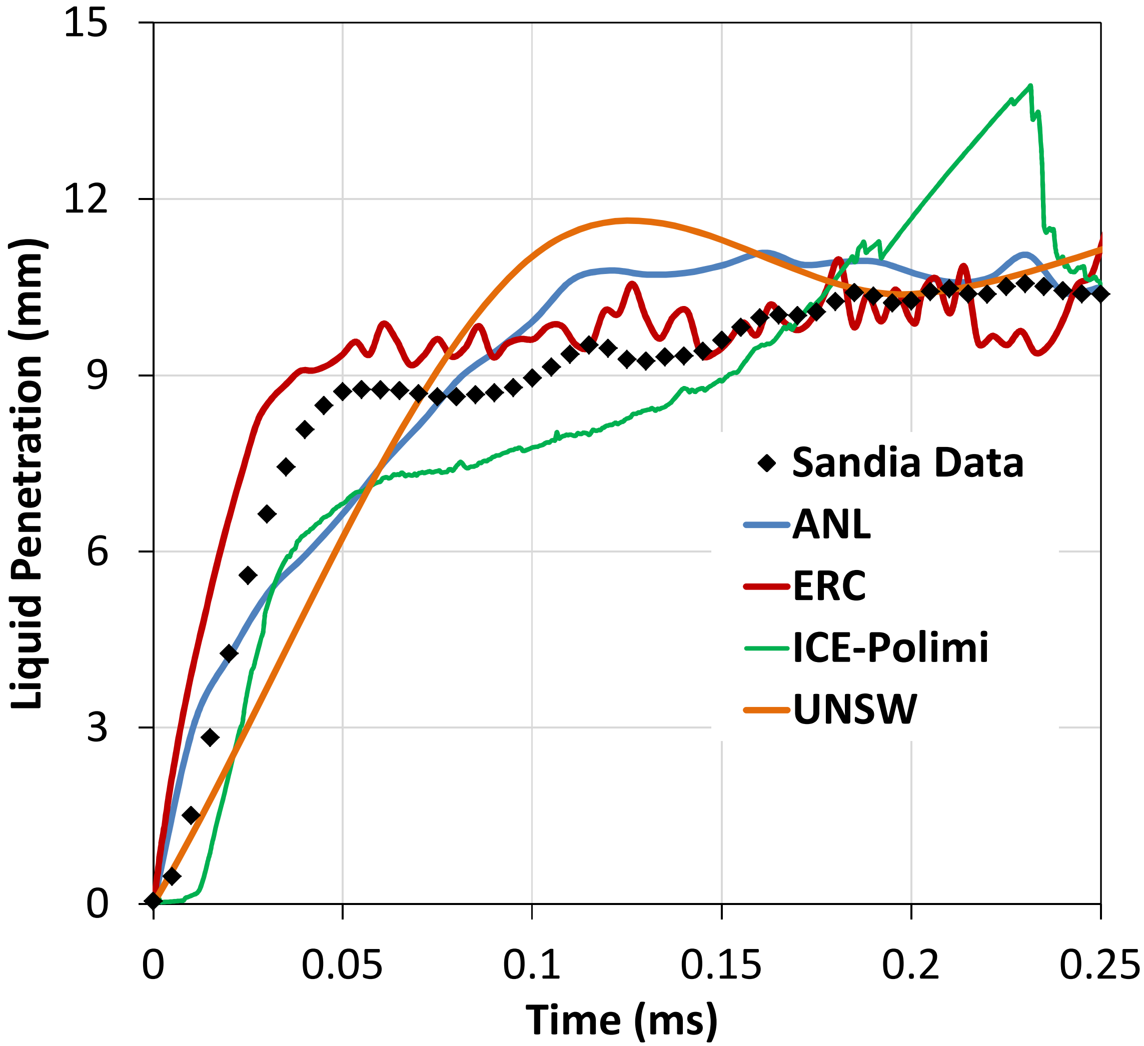
Spray Penetration vs. Time



Quasi-steady liquid length predicted within ±3-4% accuracy by all models

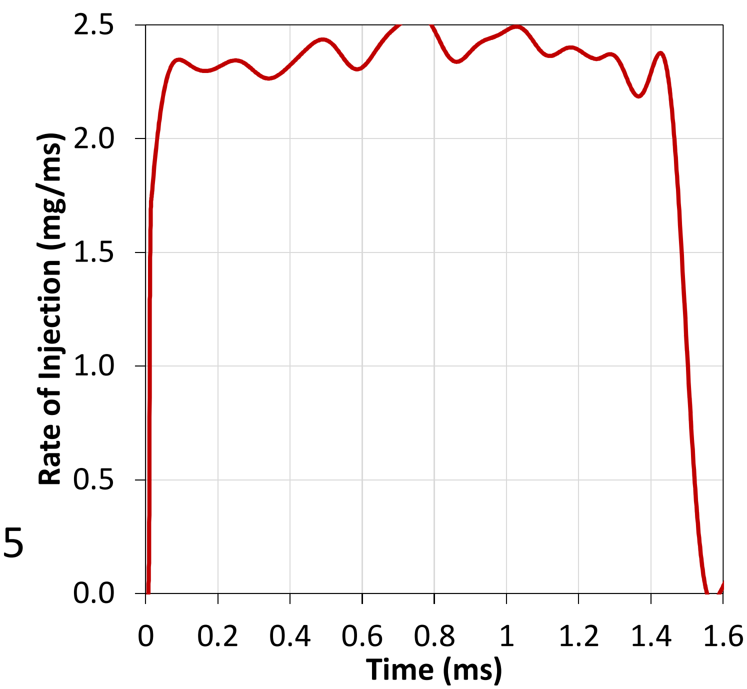
Liquid length fluctuations can be reduced by injecting higher number of computational parcels

Spray Penetration vs. Time

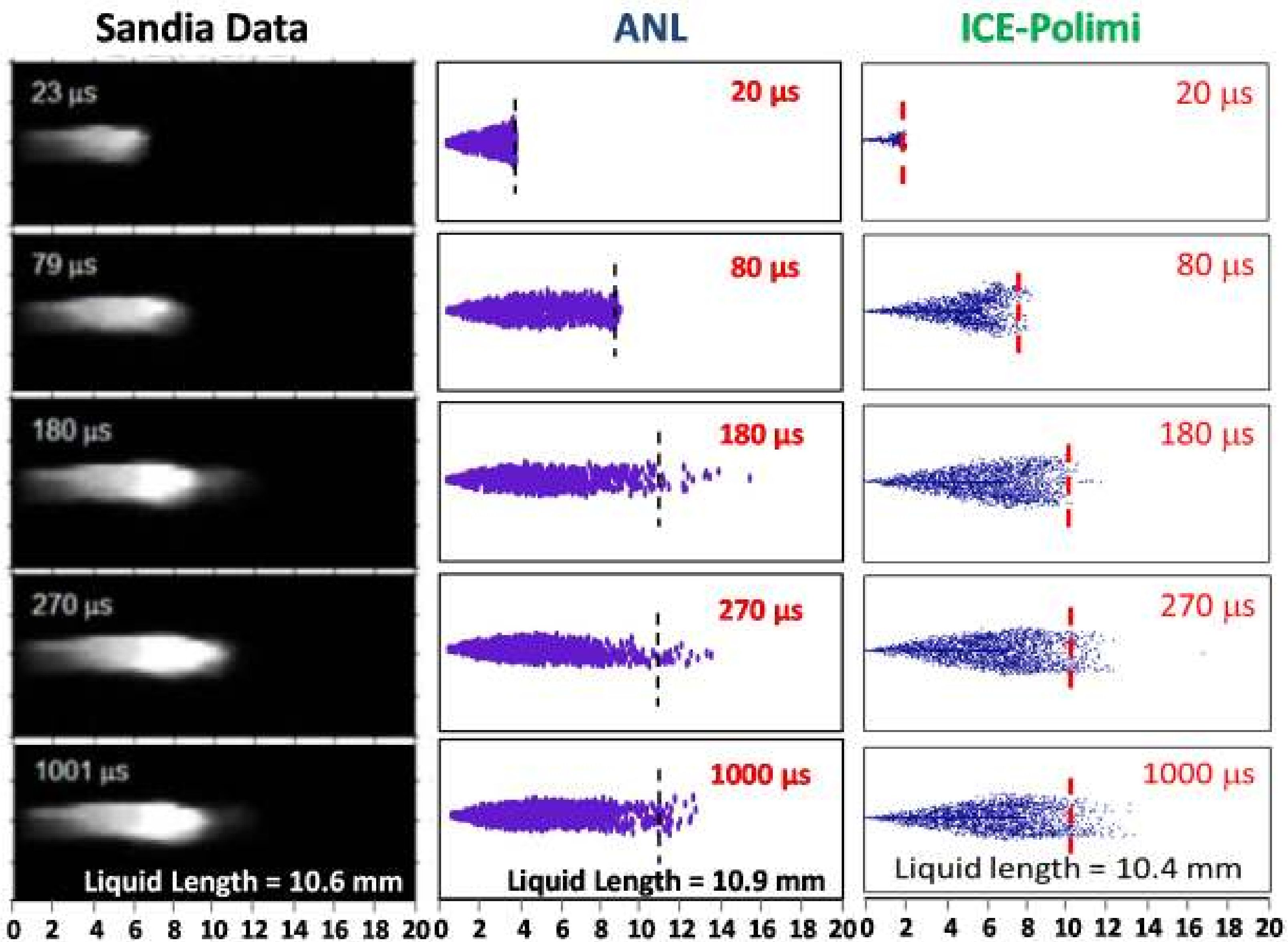


Initial transience not well predicted by any model. Possible causes:

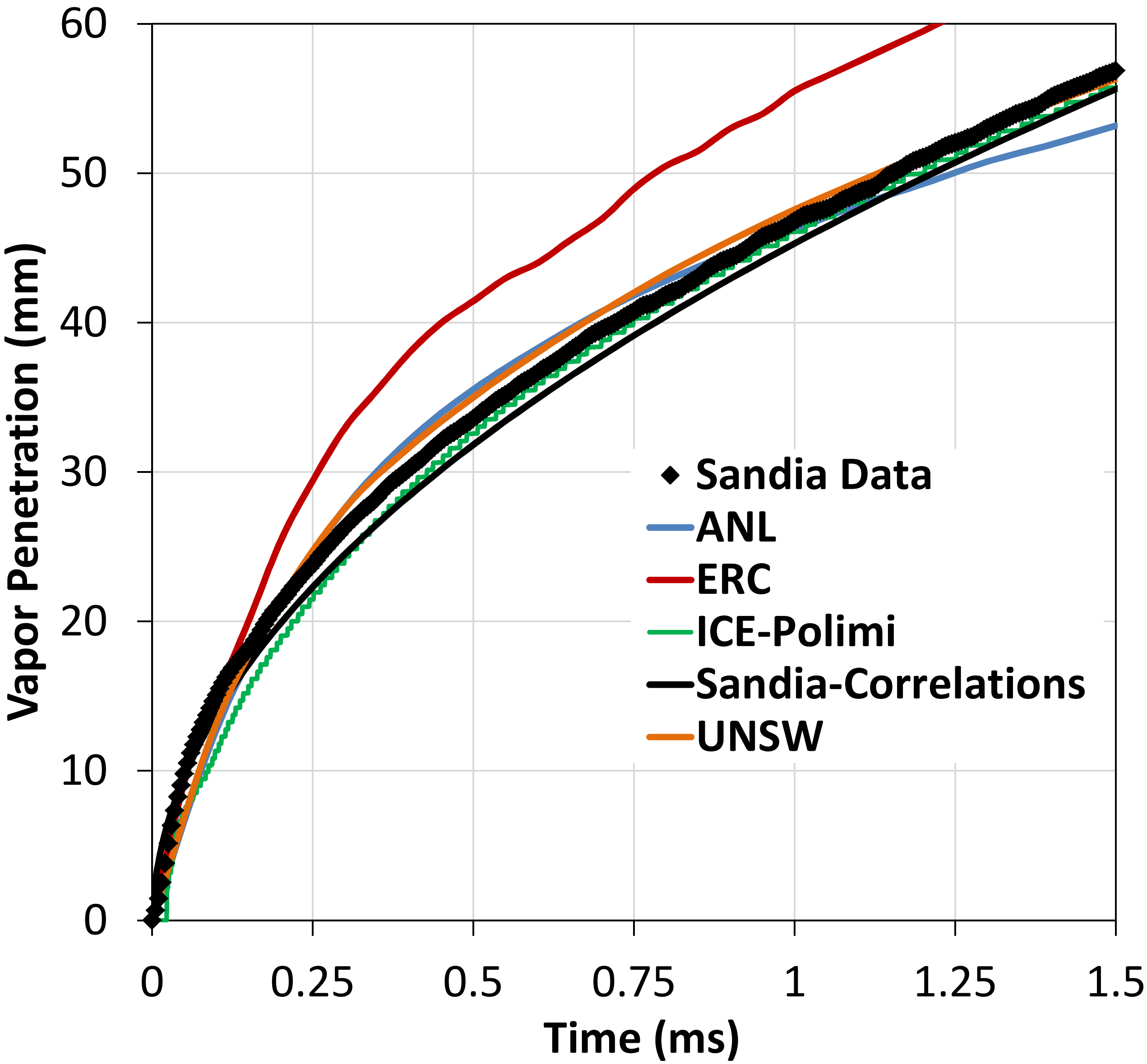
- Accurate representation of ROI?
- Need to account for nozzle geometry and needle-lift effects?

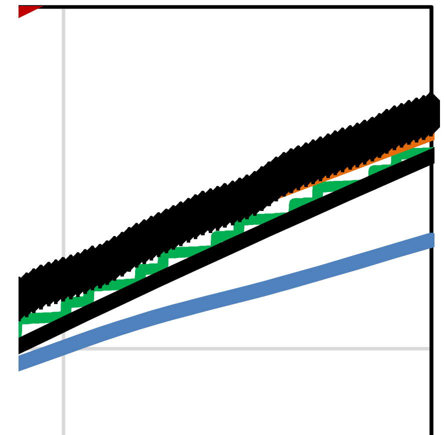


Liquid Spray Structure

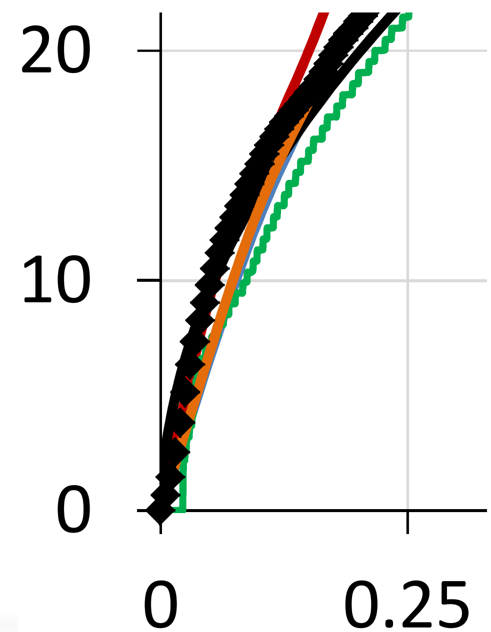


Vapor Penetration vs. Time

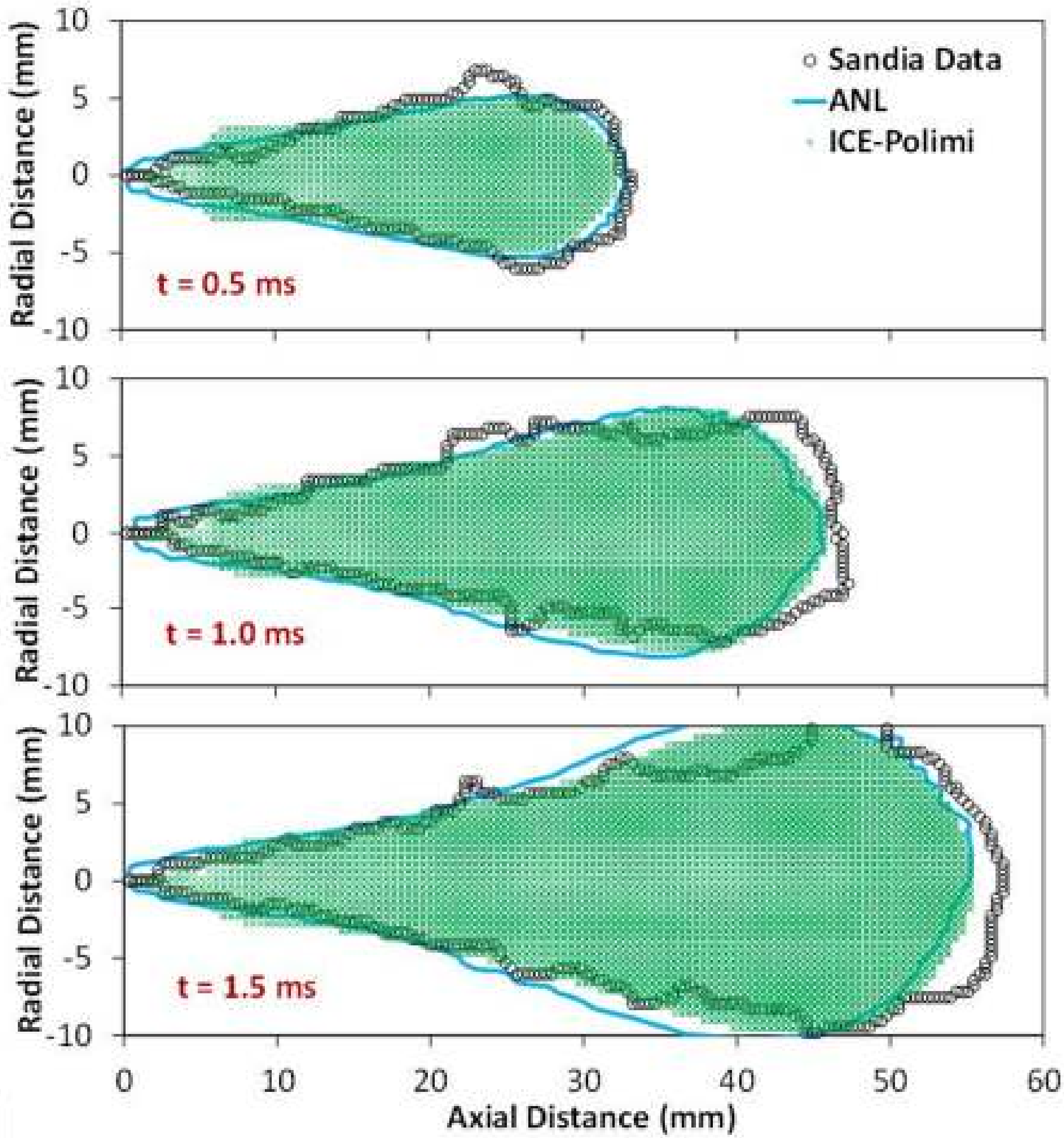




In general, the CFD models are unable to match the slopes



Vapor Boundary Comparison

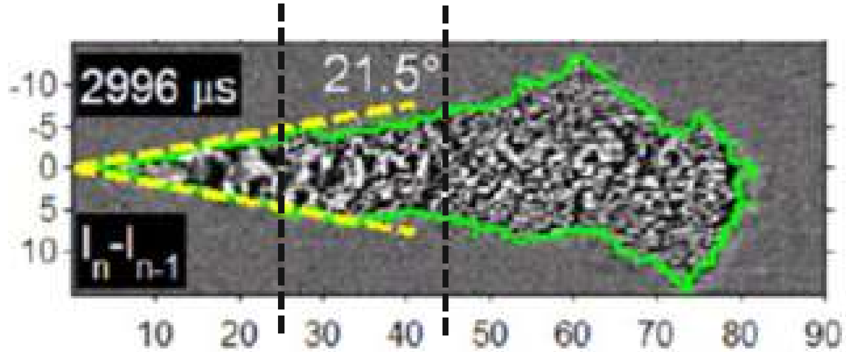


After 1.0 ms it is clear that the simulations are under-predicting vapor penetration

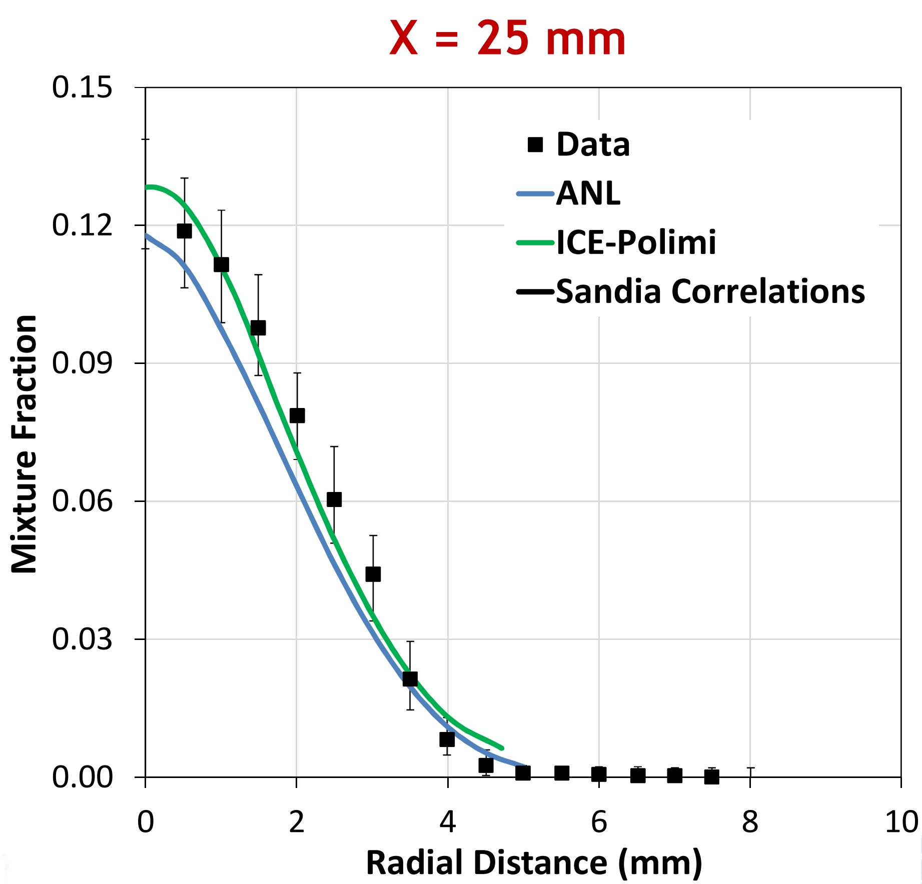
Hence, it is not surprising that both the CFD models are over-predicting the vapor dispersion, especially at 1.5 ms

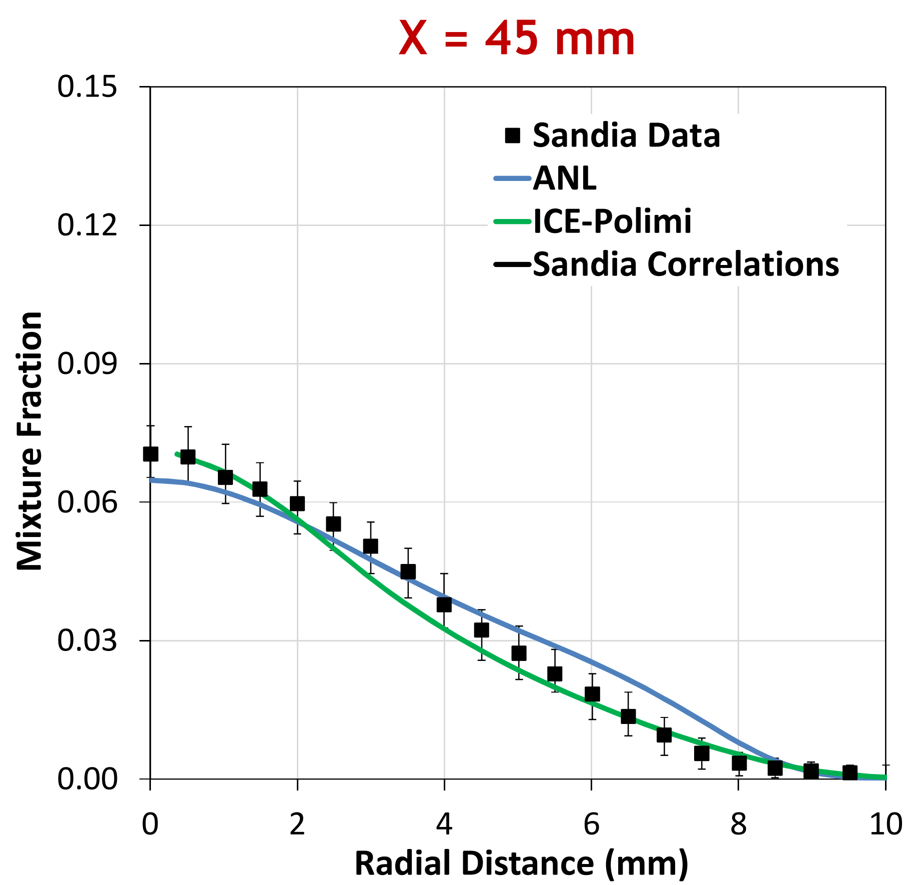
Probably a LES model can better predict the instantaneous structure of the spray

Radial Mixture fraction Distribution



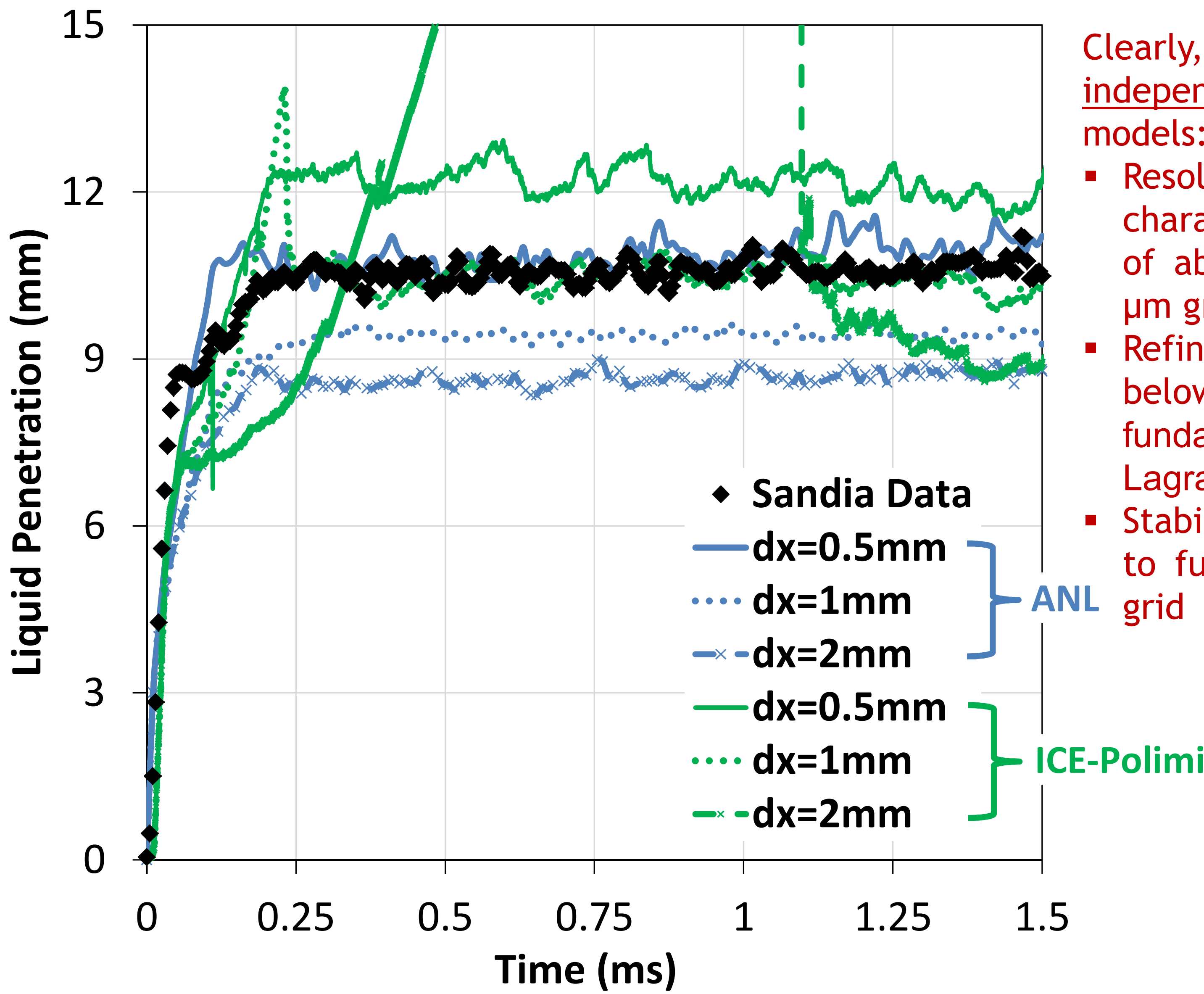
- Simulations plots at 1.5 ms
- In general, Gaussian mixture fraction profiles are well-predicted by all models at both axial locations
- Mixture fraction distribution along the center line need to be compared





Effect of “Grid” Size

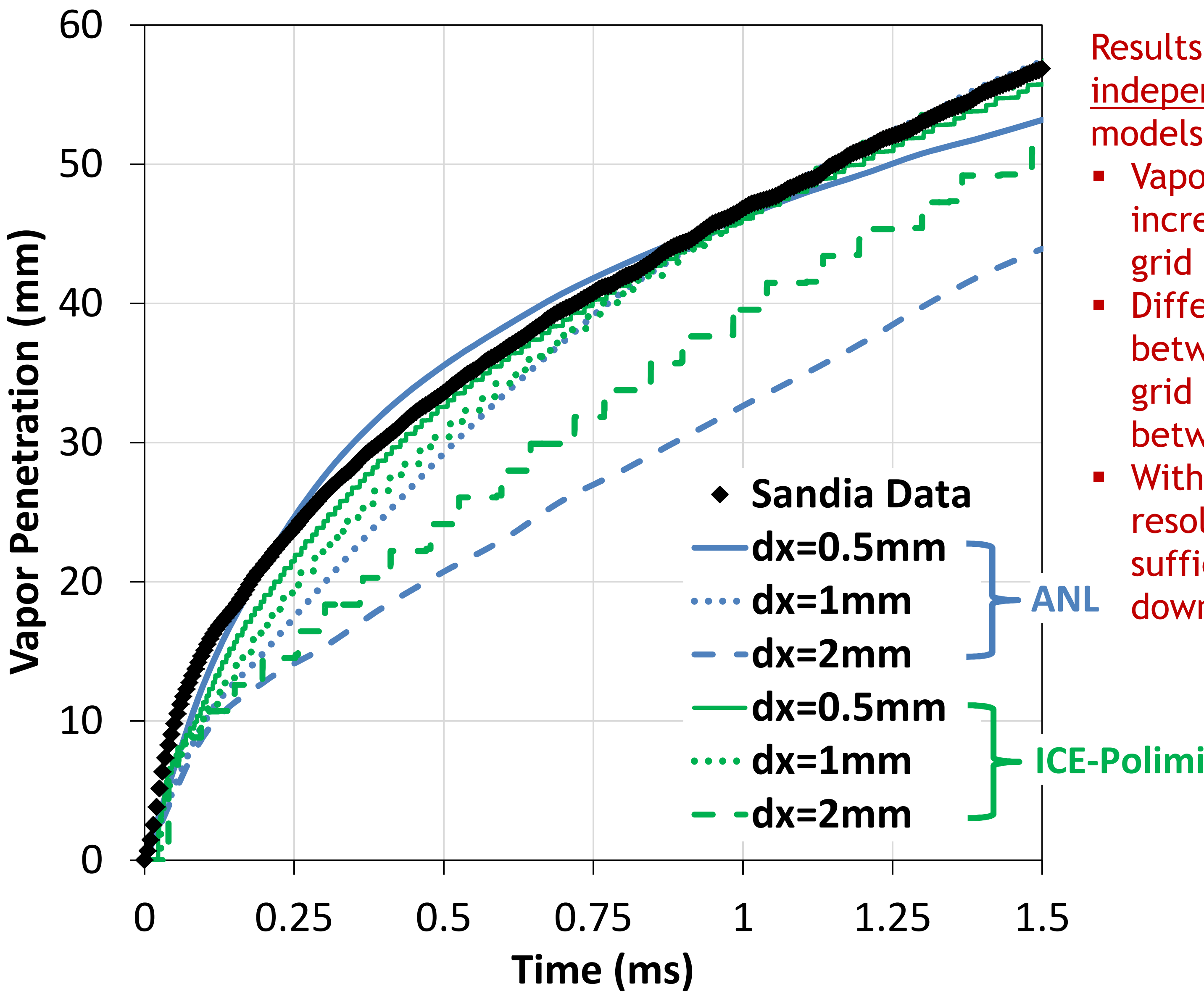
Spray Penetration



Clearly, results are <u>not grid-independent</u> with the RANS models:

- Resolving a flow with characteristic length scale of about 90 µm with 500 µm grid sizes
- Refining the grid size below 125 µm may violate fundamental Eulerian-Lagrangian assumptions
- Stability issues arise due to further refining of the grid

Vapor Penetration

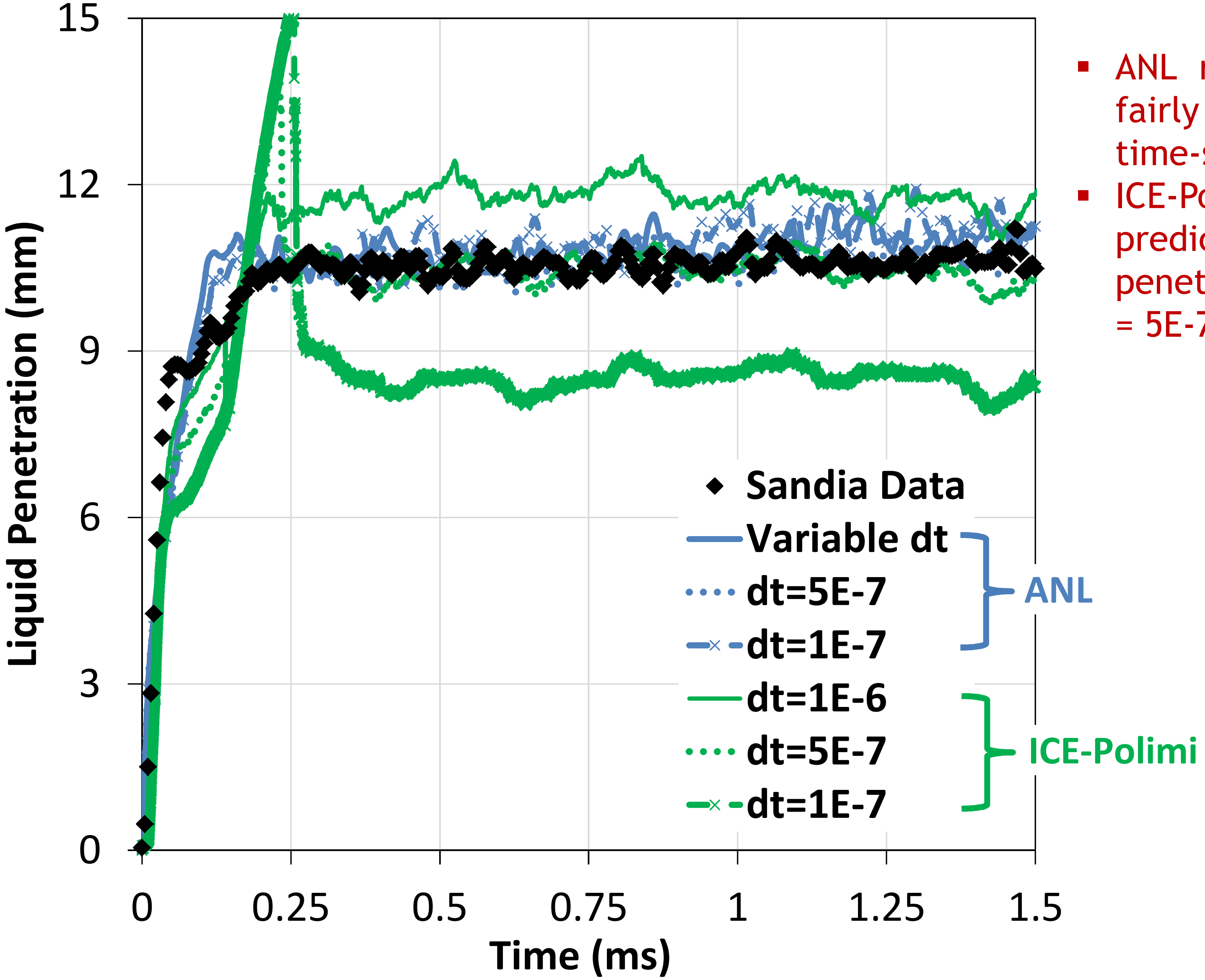


Results are not grid-independent with the RANS models:

- Vapor penetration increases with decrease in grid size
- Difference in prediction between 0.5mm and 1mm grid sizes in smaller that between 1mm and 2mm
- With adaptive mesh resolution, was the grid sufficiently resolved downstream?

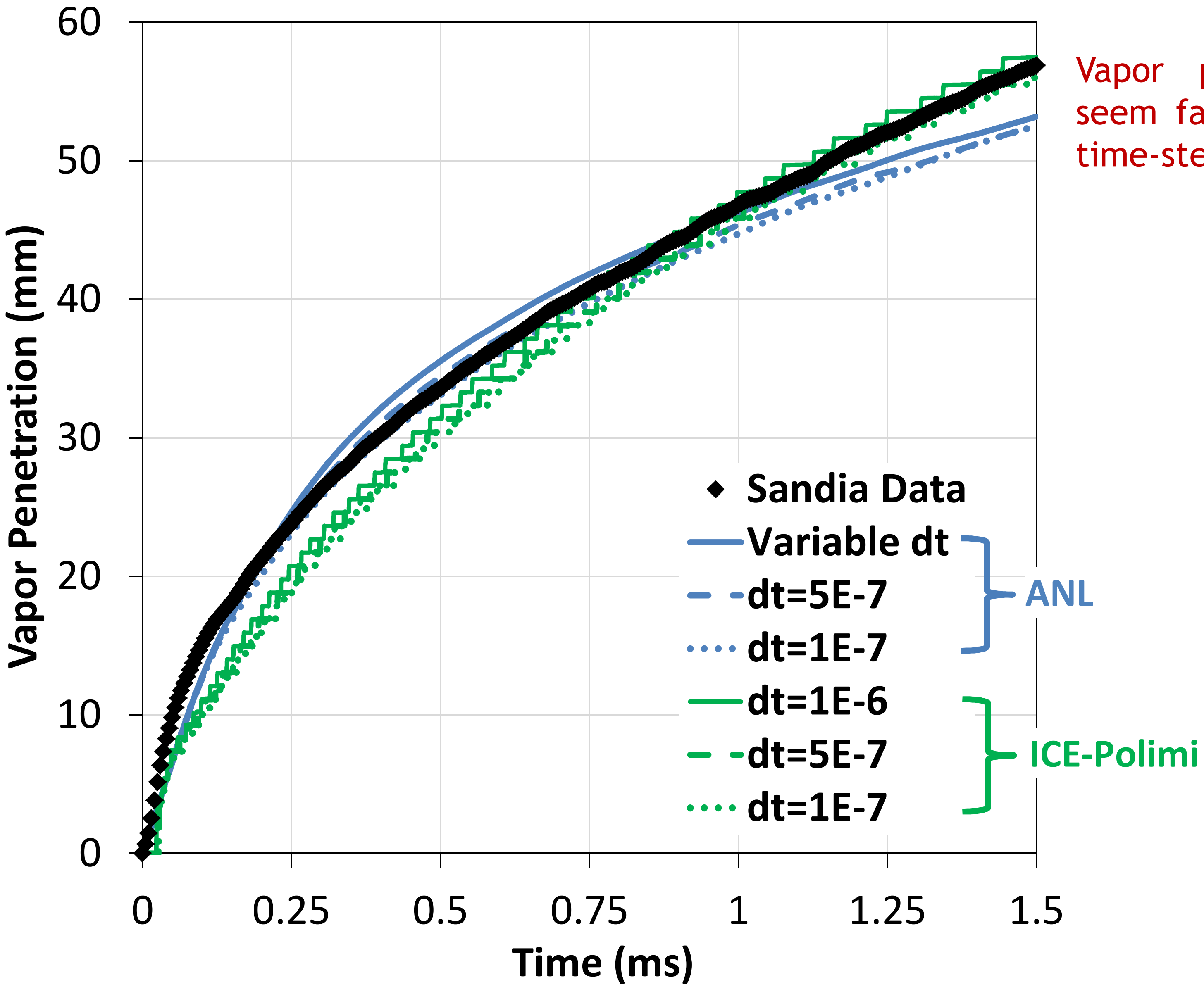
Effect of “time-step” Size

Spray Penetration



- ANL results seem to be fairly independent of time-step size
- ICE-Polimi simulations predict accurate liquid penetration values for dt = 5E-7

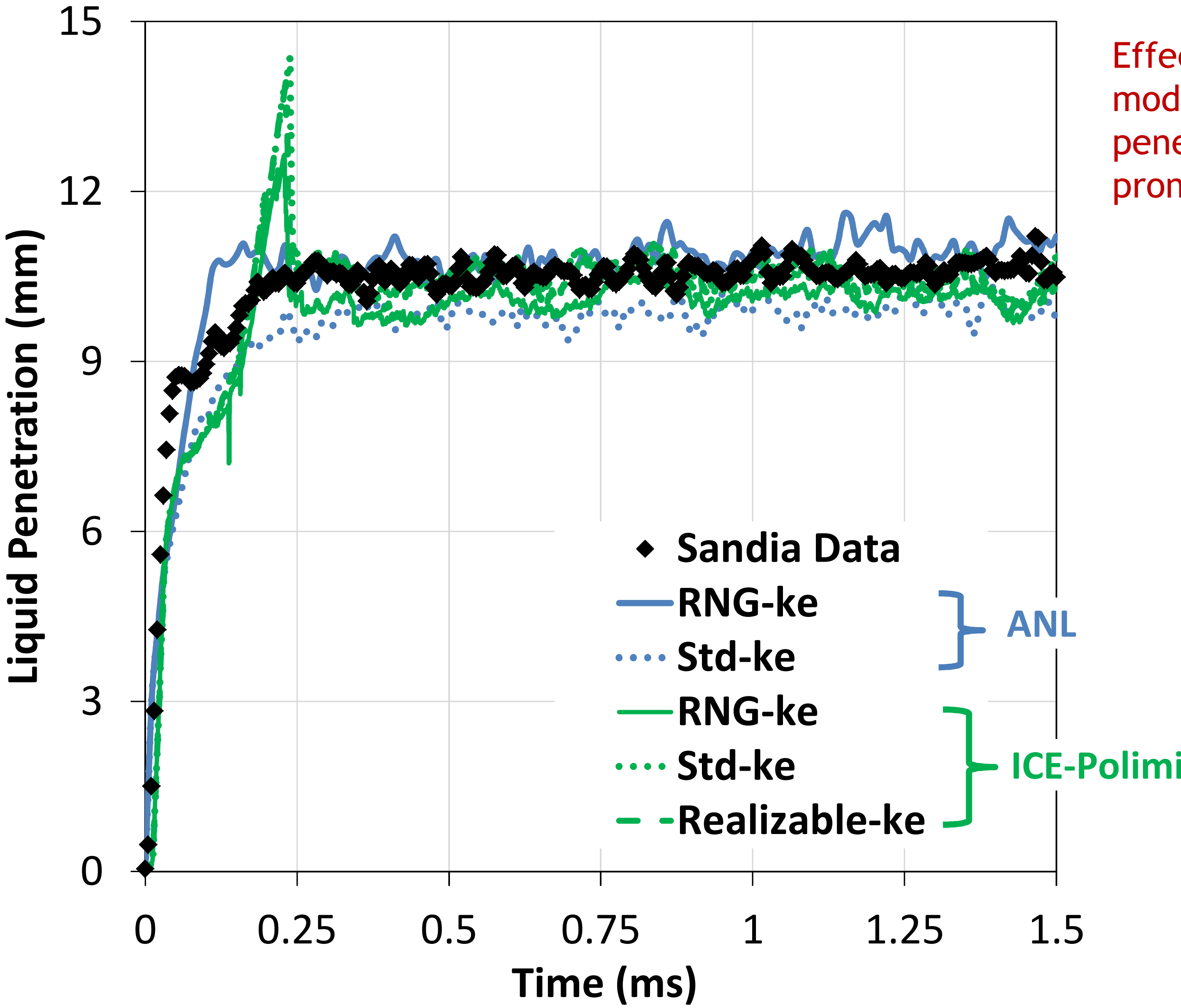
Vapor Penetration



Vapor penetration results seem fairly independent of time-step size!

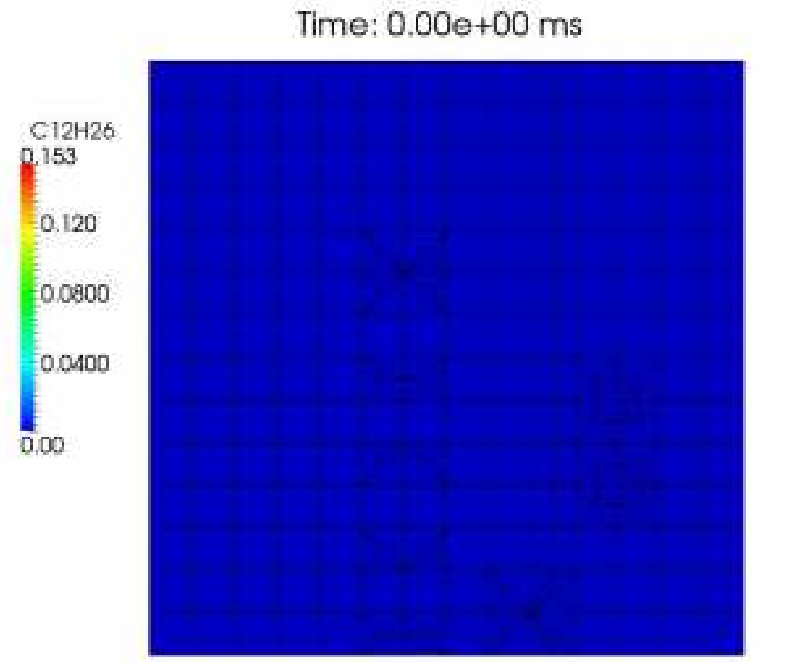
Effect of “Turbulence” Models

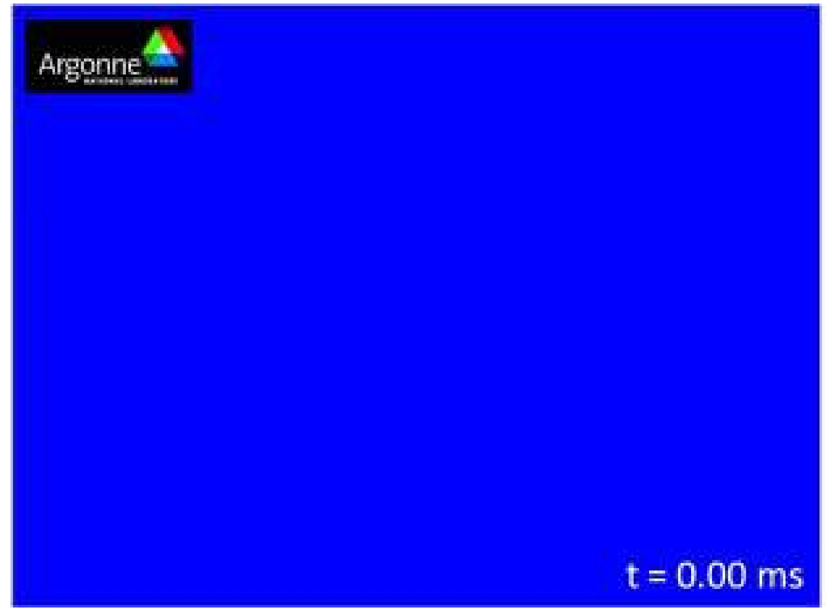
Spray Penetration: Different RANS models



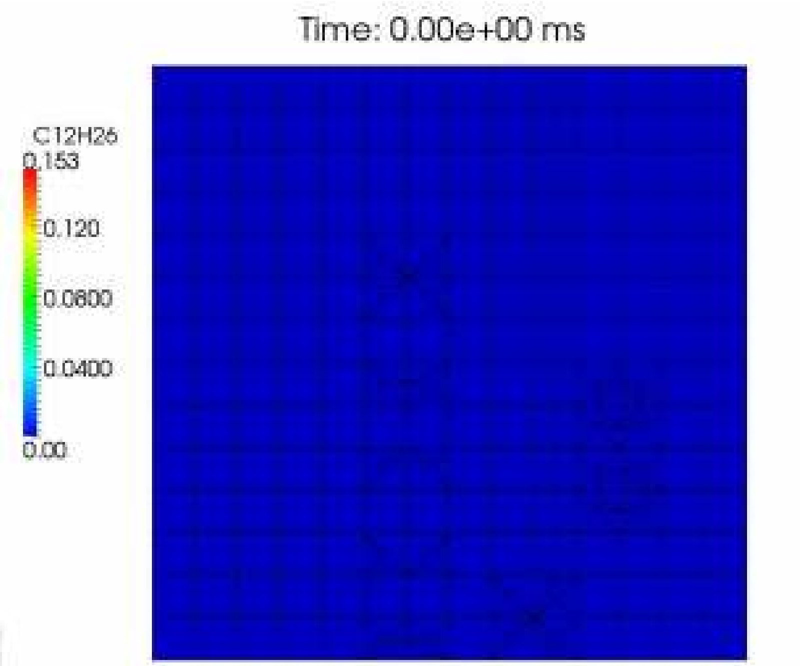
Effect of RANS turbulence models on spray penetration is not pronounced!

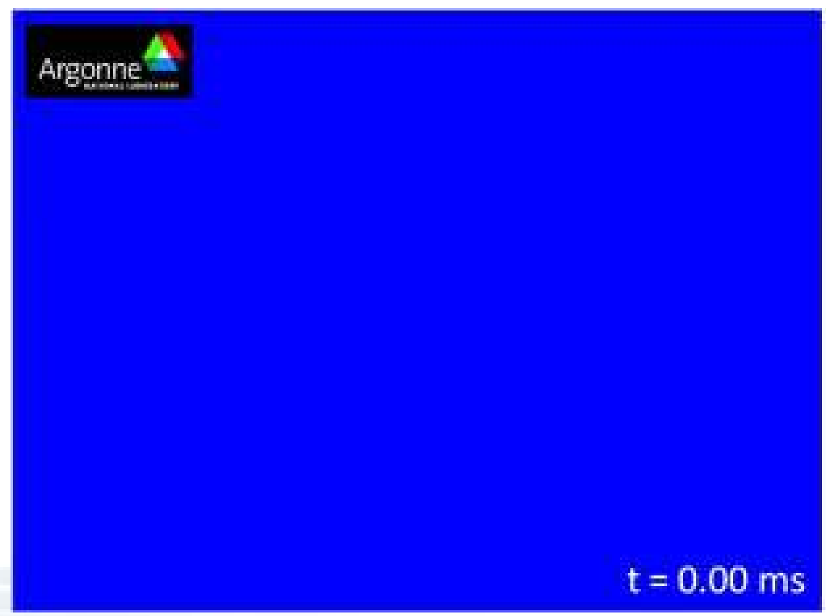
Standard k-ε



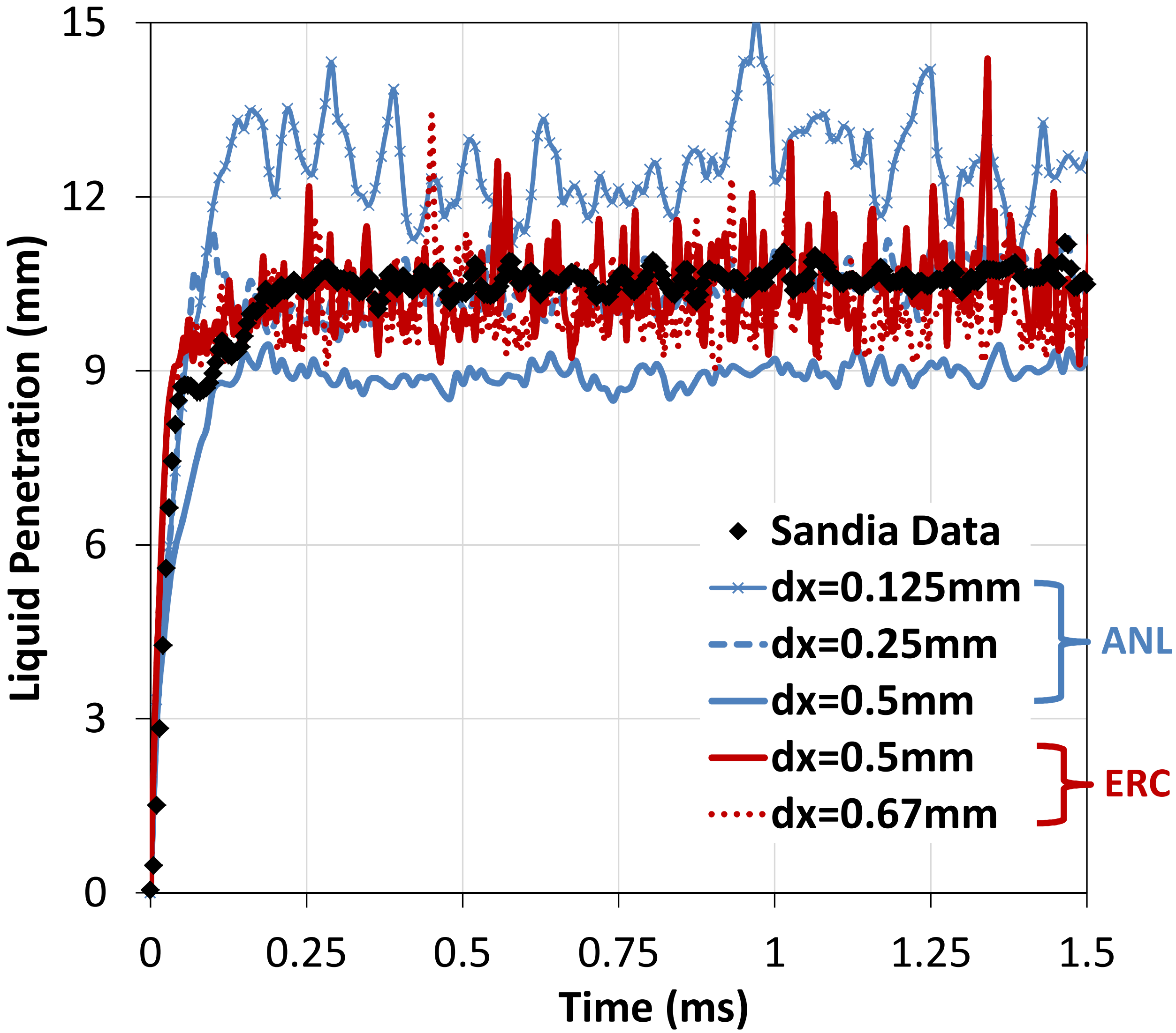


RNG k-ε





Spray Penetration: Different LES models

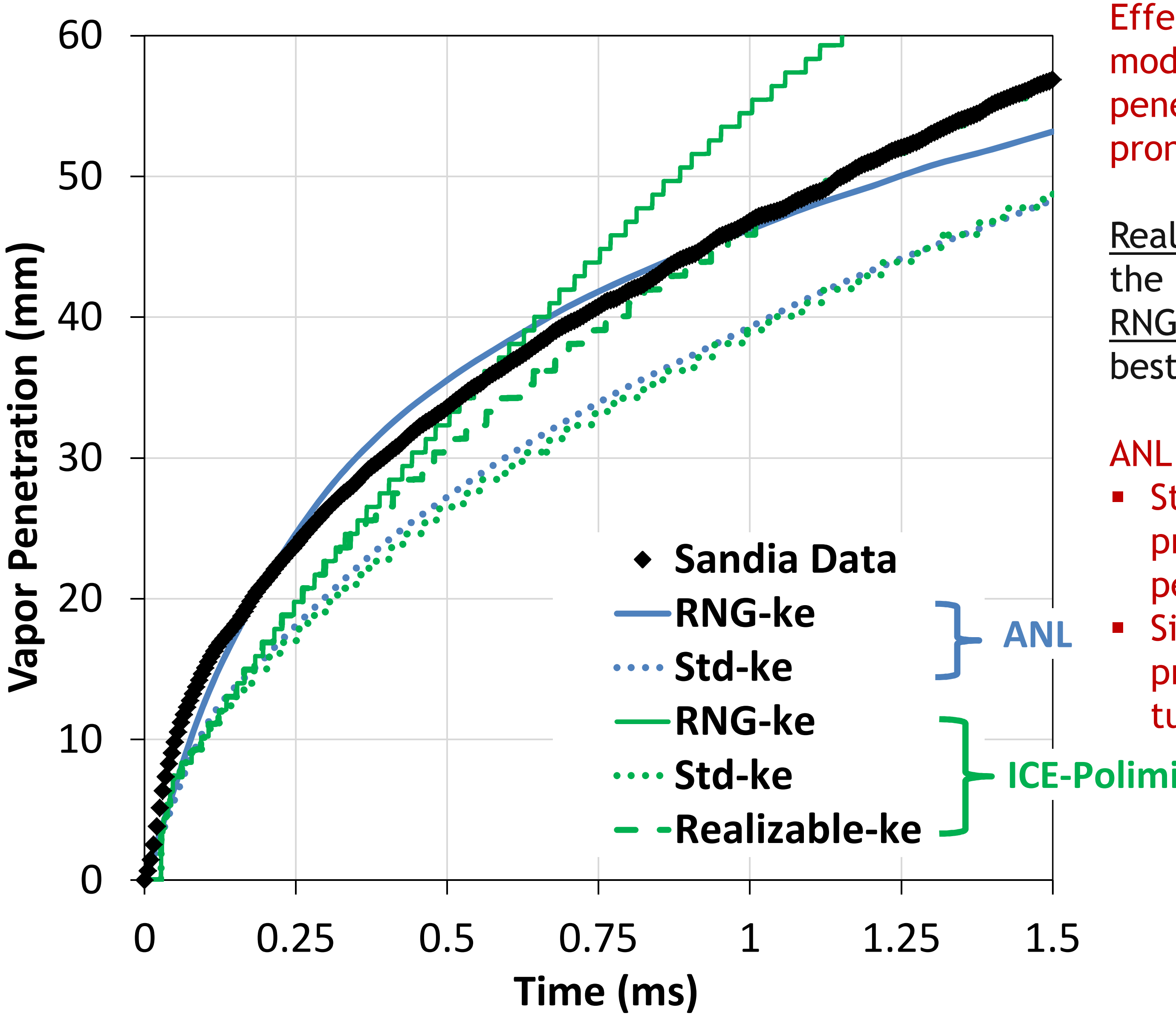


Grid independence on spray penetration observed with ERC-LES model

ANL model:

- Spray penetration increases with decrease in grid-size
- dx=0.25mm does the best job in predicting spray penetration

Vapor Penetration



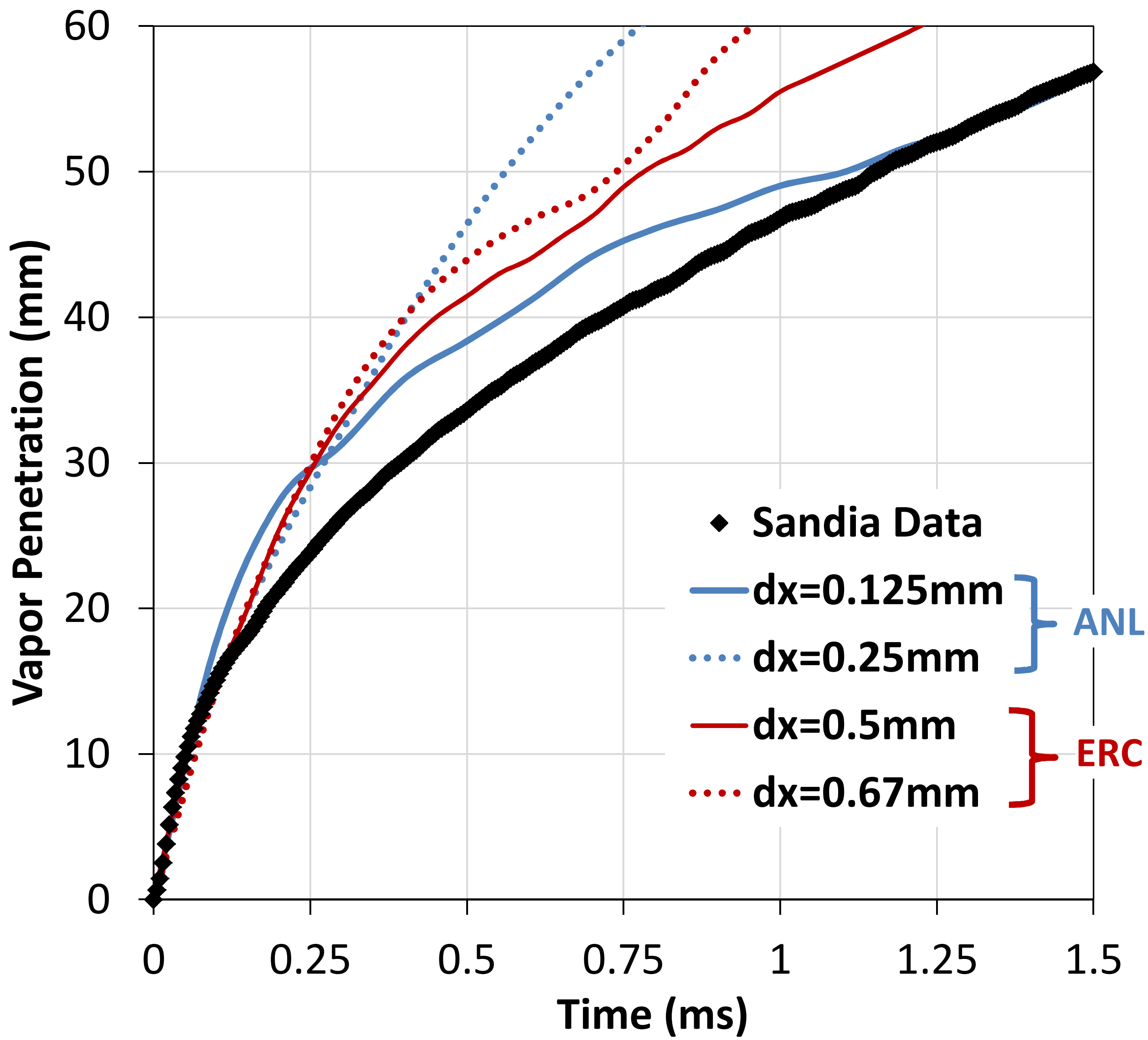
Effect of RANS turbulence models on vapor penetration is much more pronounced

Realizable k-ε model does the best job for ICE-Polimi
RNG k-ε model does the best job for ANL

ANL vs. ICE-Polimi

- Standard k-ε model predicts similar vapor penetration
- Significant difference in predictions of RNG k-ε turbulence models

Vapor Penetration

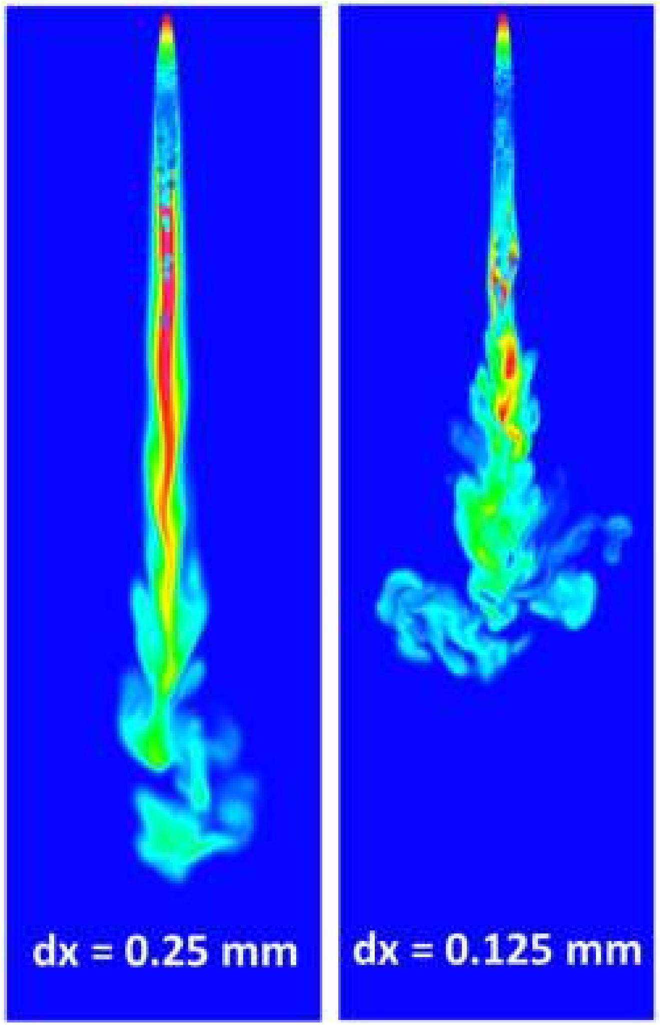


Results are <u>not grid-independent</u> with the LES models also:

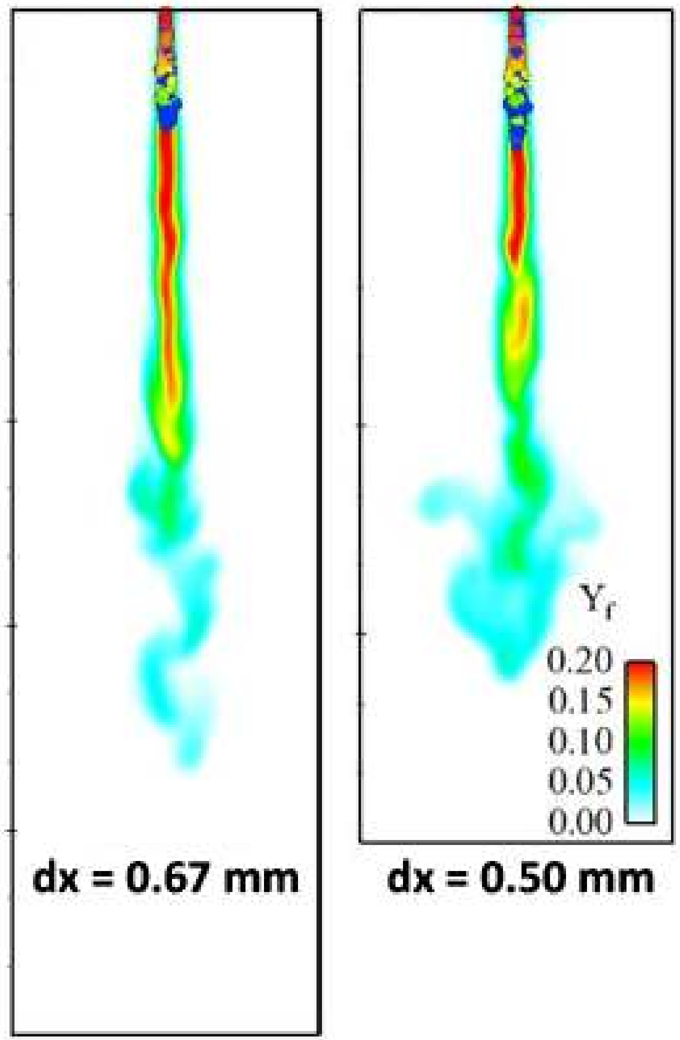
- Vapor penetration decreases with decrease in grid size. This trend is opposite to that observed for RANS simulations
- LES models need to be improved to better predict vapor penetration

Fuel Mass fraction distribution

ANL



ERC*



Smaller grid sizes results in earlier initiation of instabilities at the vapor-air interphase which results in faster breakup and reduction in vapor penetration!

Further Comparison of Computational Approaches

Test Condition Set-up

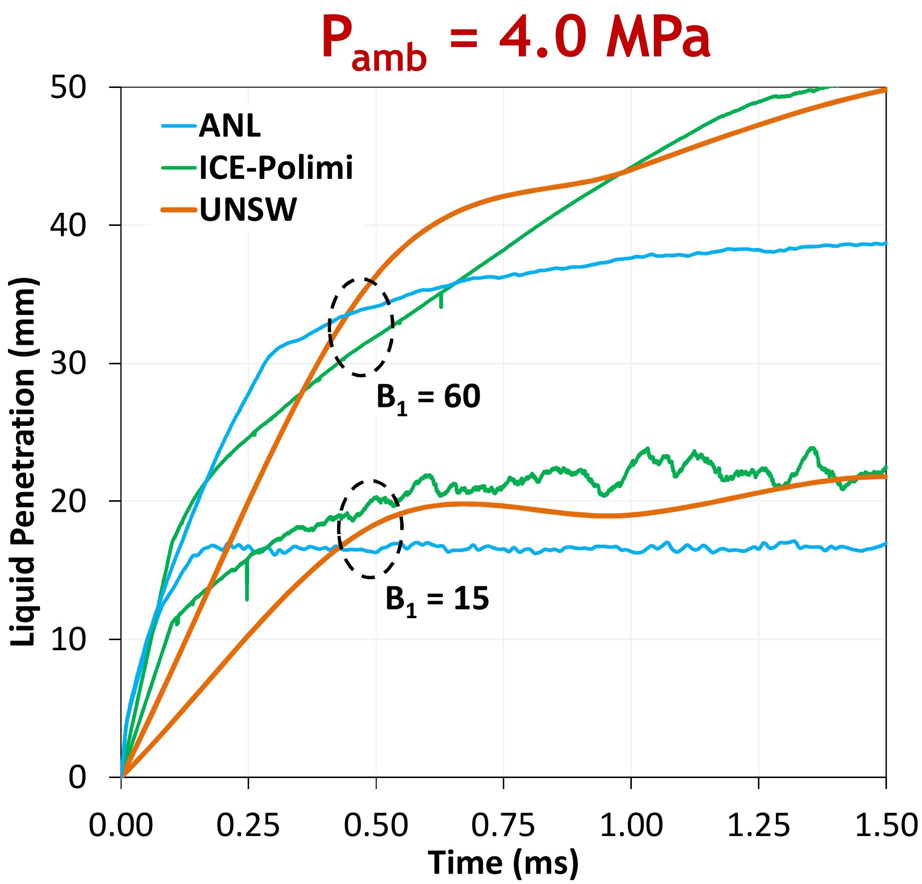
	Case 1	Case 2
Ambient gas pressure	4.0 MPa	8.0 MPa
Ambient gas density	14.8 Kg/m^3 (approx.)	30.0 Kg/m^3 (approx.)

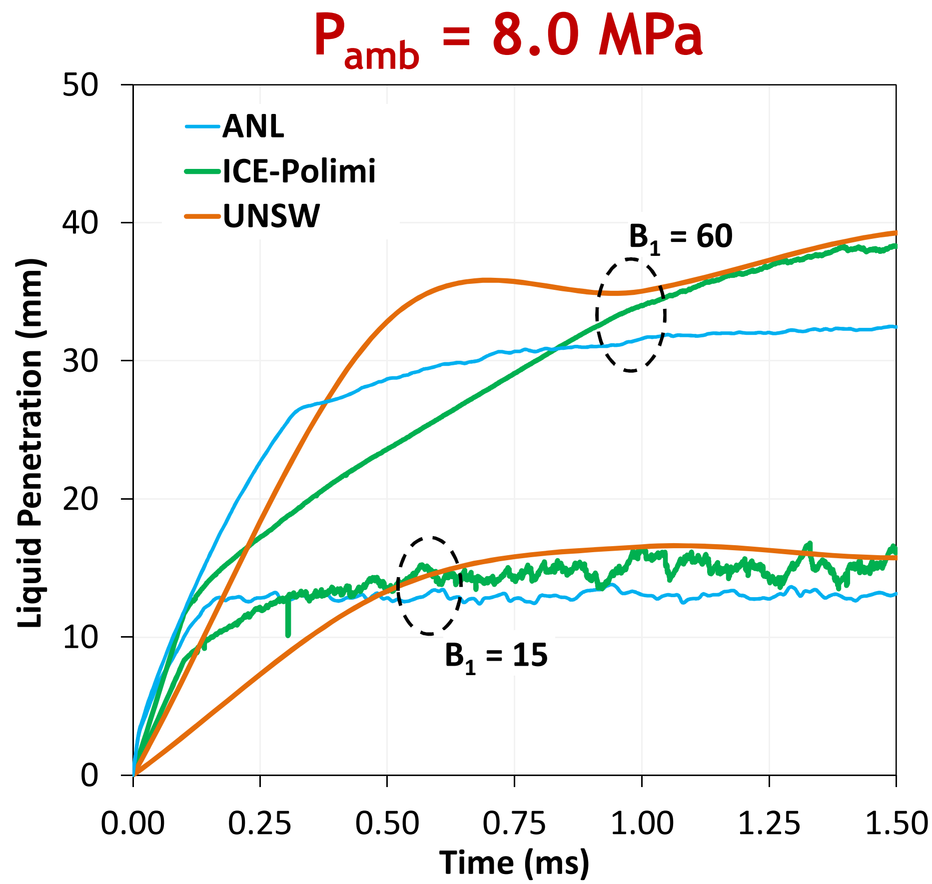
- ❑ Standard k-ε model
- ❑ Blob injection model
- ❑ No collision model
- ❑ Standard drag model
- ❑ PISO time discretization
- ❑ Frossling evaporation model

- ❑ No break-up length concept
- ❑ No turbulent dispersion
- ❑ Minimum grid size = 0.5 mm
- ❑ Fixed time-step size = 5E-7
- ❑ Wave secondary breakup model
  - ✓ B_1 = 15, 60 (KH model time-constant)

	ANL	ICE-Polimi	UNSW
Parcels injected	75,000	10,000	100,000
Initial TKE, TDR	5, 5000	0.735, 5.67	1, 1.3
Schmidt number	0.9	0.7	0.9
N.O cells at 1.5ms	35,000	18,350	6,300
Run time till 1.5ms	18 minutes on 8 processors	2.65 minutes on 6 processors	85 minutes on 2 processors

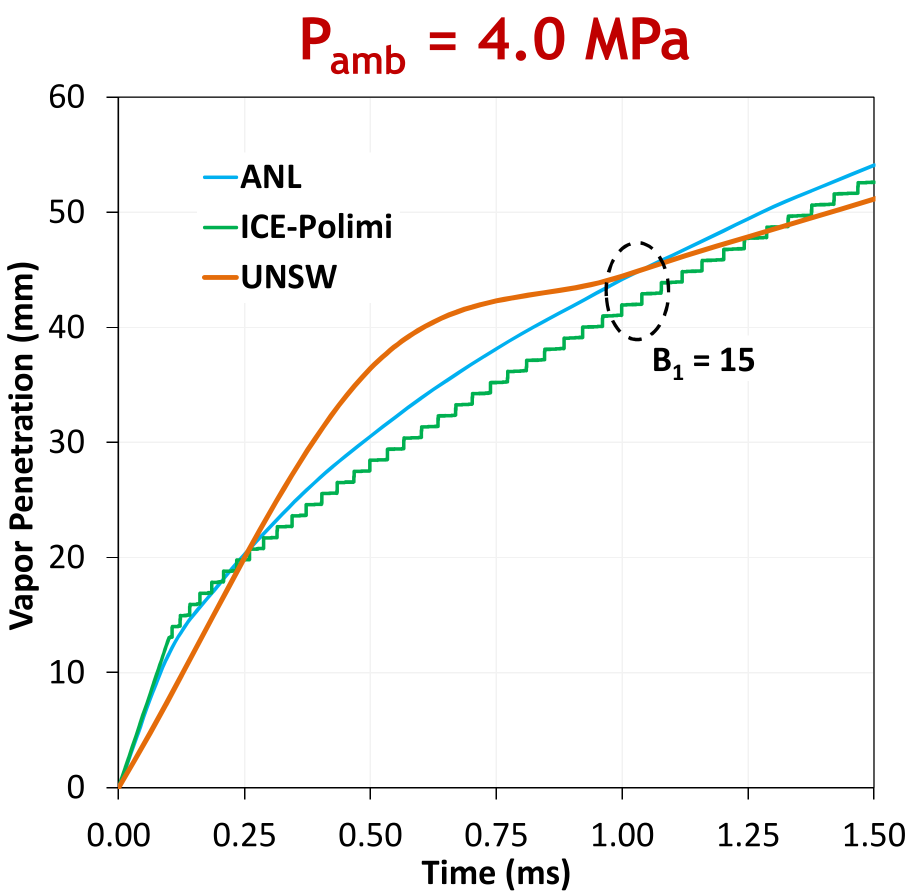
Spray Penetration

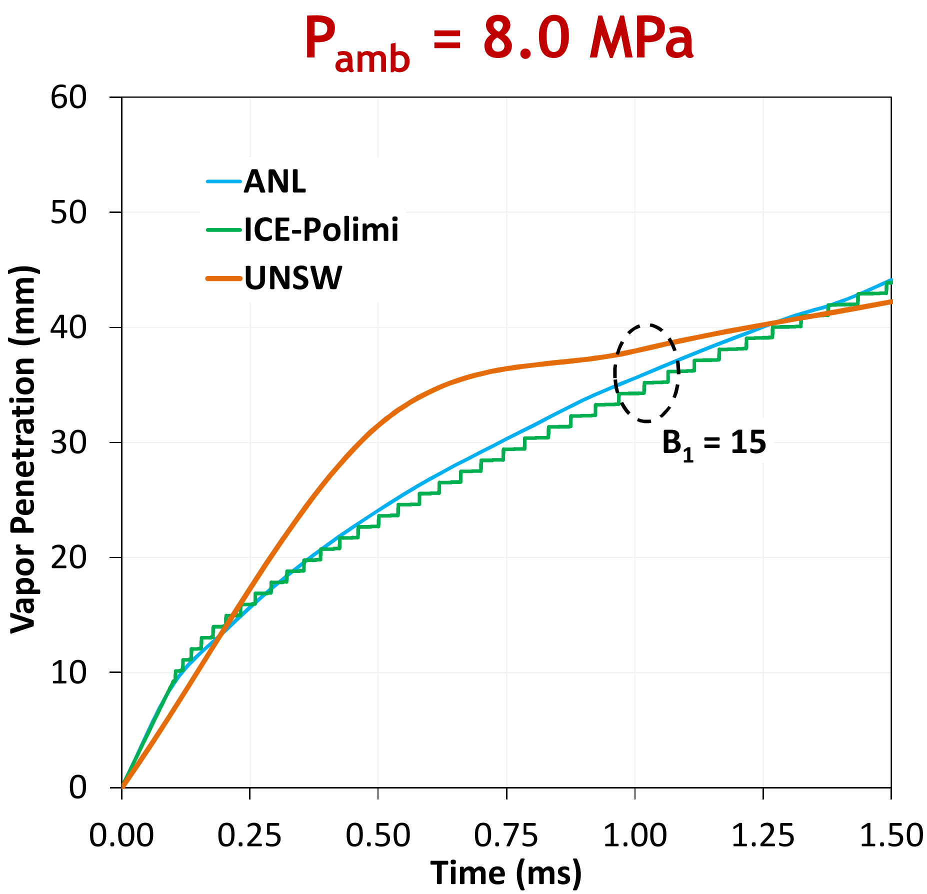




- B1 is perhaps the most influential spray model constant
- Differences in simulation results are very apparent
  - Initial transience is markedly different
  - Different steady state liquid lengths predicted
  - Differences are more pronounced at lower ambient pressure values

Vapor Penetration





- Differences in simulation results for vapor penetration are less pronounced
  - In fact, ANL and ICE-Polimi results are very close to each other which is very surprising, given the differences in liquid penetration

References

- LM Pickett, CL Genzale, G Bruneaux, LM Malbec, L Hermant, C Christiansen, J Schramm. Comparison of Diesel Spray Combustion in Different High-Temperature, High-Pressure Facilities. SAE 2010-01-2106
- LM Pickett, J Manin, CL Genzale, DL Siebers, MPB Musculus, CA Idicheria. Relationship between diesel fuel spray vapor penetration/dispersion and local fuel mixture fraction. SAE 2011-01-0686
- http://www.sandia.gov/ecn/

- G D'Errico, T Lucchini. Validation of spray and combustion models for diesel engines using constant-volume experiments. ILASS 2011

- Nidheesh Bharadwaj. Large eddy simulation turbulence modeling of spray flows. PHD thesis, University of Wisconsin-Madison, 2010

Discussions

Decide on future cases to run for “apples-to-apples” comparison and validation:
1) Grid size
2) Breakup model
3) Turbulence model (RANS vs. LES)
4) Chemical-kinetic mechanism

Experimental data of interest:
1) Rate of injection measured with different techniques such as x-ray radiography, Bosch rate-meter, momentum flux methods.
   Ramirez et al., “Quantitative X-ray measurements of high-pressure fuel sprays from a production heavy duty diesel injector” Experiments in Fluids (47) 119-134, 2009