ECN Workshop 1 – Spray A Modeling

Group Coordinator: Sibendu Som (Argonne National Laboratory)

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Nidheesh Bharadwaj, Noah Van Dam, Chris Rutland* (University of Wisconsin - UW),
Gianluca D'Errico*, Tommaso Lucchini, Daniele Ettore (Politechnico di Milano - Polimi),
Lyle Pickett* (Sandia National Laboratory - Sandia),
Yuanjian Pei*, Evatt Hawkes, Sanghoon Kook (University of New South Wales - UNSW)

Summary of Spray A modeling session

The primary objective of the Spray A modeling session was for different modelers to use their best practices in matching the spray A non-reacting data. The non-reacting data used for validation included liquid spray penetration vs. time, vapor penetration vs. time, mixture fraction vs. radial position at a given time, location of vapor and liquid boundaries at different times. Four different codes were used namely: CONVERGE (ANL), KIVA-3V (UW), OpenFOAM (Polimi) and FLUENT (UNSW). In addition, 1D correlations developed at Sandia were used to predict vapor penetration and mixture-fraction distribution. The group leaders of each modeling group gave a short presentation of their modeling approach and numerical parameters used. All the simulation approaches adopted the Lagrangian approach for the spray modeling.

The group coordinator then summarized all results from different research groups. Parametric studies were performed to quantify the influence of grid size, time-step size, and turbulence models on liquid and vapor penetration vs. time. It should be noted that the definition of liquid length and vapor penetration was different for various modeling approaches. Different turbulence models tested included RANS (standard k-ε, realizable k-ε, and RNG k-ε) and LES models (such as Smagorinsky and dynamic viscosity). Further, in order to facilitate apples-to-apples comparison, simulations with same minimum grid size, similar time-step size, models, and model constants were performed with CONVERGE, OpenFOAM, and FLUENT.

Conclusions

1) Liquid penetration: The quasi-steady liquid length was well predicted within 3-4% accuracy by all the models despite differences in modeling approaches and definitions. Liquid spray boundaries were well captured by ANL and Polimi models. However, initial transience was not well captured by any of the modeling approaches.
2) Vapor penetration: Vapor penetration was fairly well captured by all the simulations, UNSW probably doing the best job. In addition, ANL and Polimi were able to capture the location of vapor boundaries very well at 0.5 and 1ms. However, at 1.5ms vapor penetration is underpredicted, consequently, spray dispersion is overpredicted.
3) Mixture fraction distribution: Sandia correlations and modeling results from ANL and Polimi captured the Gaussian mixture fraction trends well. At certain instants though the predictions were beyond the experimental error bars.
4) Effect of grid size: Simulation results are not grid independent for the grid size range studied. Spray and vapor penetration increase with a decrease in grid size for the RANS models.

5) Effect of time-step size: Liquid and vapor penetration results from ANL were time-step independent. Vapor penetration results from Polimi were time-step independent, however, liquid spray penetration results were not.
6) Effect of turbulence model: Turbulence models had pronounced effects on vapor penetration while effect on liquid spray penetration was negligible. The best vapor penetration results were predicted by the RNG k-ε model using CONVERGE and realizable k-ε model using OpenFOAM. Dynamic viscosity based LES results from UW for spray penetration seemed to be grid independent. Increasingly detailed flow structures were observed with smaller grid sizes using LES models from both UW and ANL.
7) Despite differences in models, grids, and modeling approaches, different best practice approaches were able to capture experimental trends fairly well, which is not surprising. Next, a set of simulations were performed with same minimum grid size, similar time-step size, models, and model constants. Liquid and vapor penetration results revealed significant differences between ANL, Polimi, and UNSW simulations. The reasons for these differences warrant further investigations.

Discussion and Recommendations

1) Liquid penetration: Liquid length fluctuations can be reduced by injecting higher number of computational parcels. Initial transience can be better reproduced with an accurate ROI, accounting for the nozzle flow and needle lift effects, and accurate discharge coefficient values. The influence of spray model constants on this initial transience also needs to be characterized. Spray breakup model constants perhaps have the most significant influence on spray penetration.
2) Vapor penetration: Modelers need to focus on the early and late parts of vapor penetration profiles where discrepancy with experimental data is the largest. This may improve the spray dispersion predictions also.
3) Mixture fraction distribution: This is a difficult parameter to match. Future studies should focus on matching the mixture fraction decay along the centerline also.
4) Full 3-D simulations will probably be more accurate than 2-D simulations.
5) The location of the modeled injector exit in the mesh should be stated by modelers (e.g. are drops injected from the center of a cell or from a cell vertex?).
6) LES models need to be improved in order to better match vapor penetration and distribution.
7) The minimum grid size should be refined to 0.125mm to observe if grid independence on parameters like liquid and vapor penetration.

Future work

1) The major outcome of this session was to ensure that the next set of simulations are presented with standardized definitions of parameters like liquid and vapor penetration. Please refer to the summary sheet for the n-heptane baseline modeling session on recommendations for these definitions.
2) Spray A data was under one well-defined operating condition. Since all these models have tunable constants, matching data at one operating point is not very difficult. Parameters such as ambient temperature, injection pressure etc., need to be varied to characterize its influence on liquid and vapor penetration values. Such data will provide a more rigorous test-bed for different modeling approaches.
3) Future simulations from different groups need to employ same models, model constants, Schmidt number value, n.o. parcels injected, initial turbulence levels, grid size, time-step size etc.

4) Validation against combustion parameters such as lift-off length and ignition delay could not be performed in the absence of a reduced chemical kinetic mechanism. The session coordinator is collaborating with Lawrence Livermore National Laboratory and University of Connecticut to develop an appropriate reduced chemical kinetic mechanism for dodecane combustion. The aim is to develop a reduced mechanism consisting of 100 species or lesser for simulations.

References

1) 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.
2) 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.
3) http://www.sandia.gov/ecn/
4) G D'Errico, T Lucchini. Validation of spray and combustion models for diesel engines using constant-volume experiments. ILASS 2011
5) Nidheesh Bharadwaj. Large eddy simulation turbulence modeling of spray flows. PHD thesis, University of Wisconsin-Madison, 2010

Spray-Combustion Modeling set-up at Argonne National Laboratory

Sibendu Som, Douglas E. Longman

Engine and Emissions Group

Argonne National Laboratory

Sponsors: U.S. Department of Energy, Office of Vehicle Technology under the management of **Mr. Gurpreet Singh**

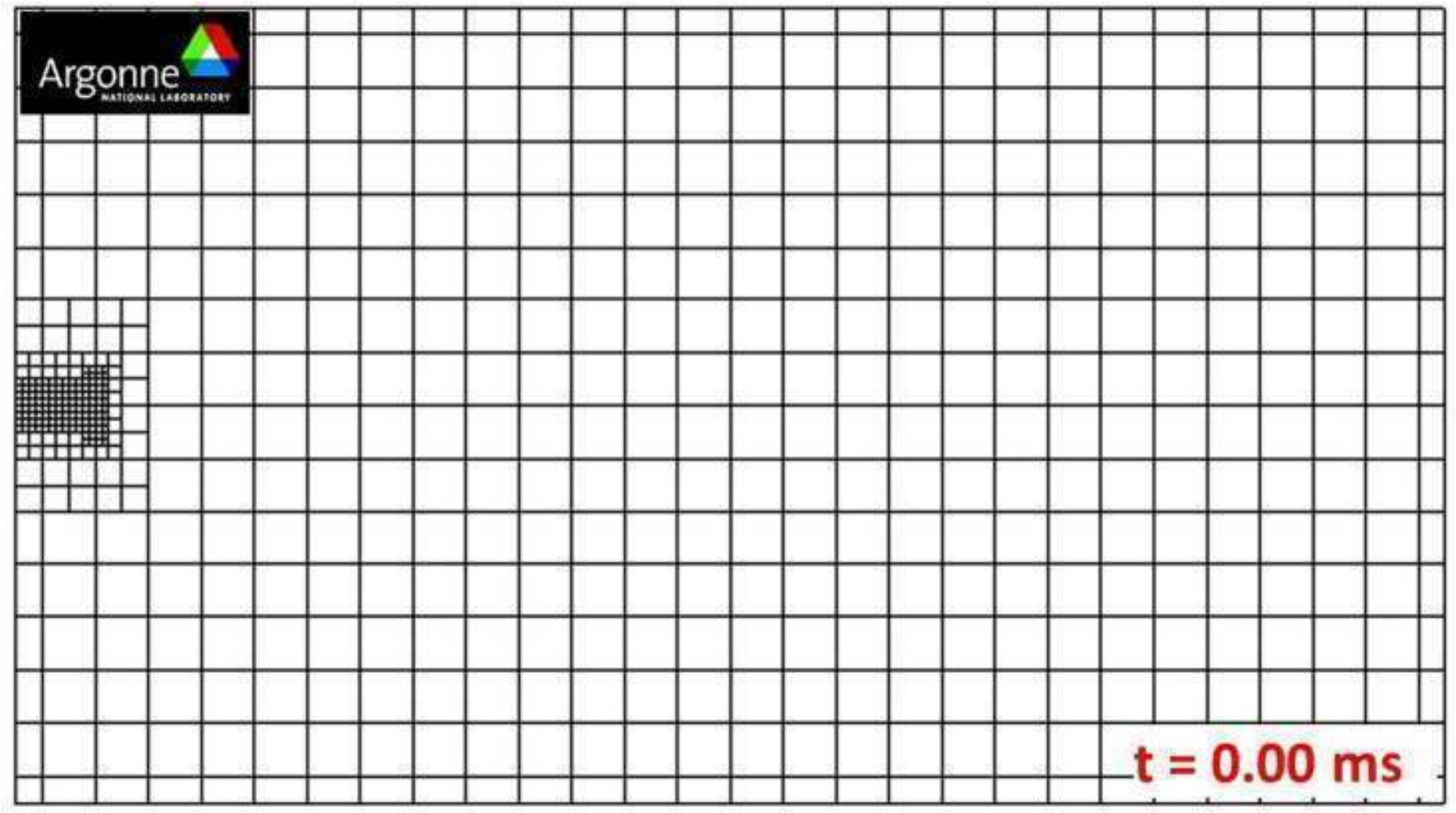
Engine Combustion Network Workshop - 1

Modeling Set-up

Modeling Tool	CONVERGE
Dimensionality and type of grid	3D, structured with Adaptive Mesh Resolution
Spatial discretization approach	2nd order finite volume
Smallest and largest characteristic grid size(s)	Base grid size: 2mm or 4mm Finest grid size: 0.125mm, 0.25mm, 0.5mm Gradient based AMR on the velocity and temperature fields. Fixed embedding in the near nozzle region to ensure the finest grid sizes
Total grid number	30K-40K for 0.5mm – RANS simulations (Non-reacting) 1.3 million for 0.125mm – LES case (Reacting) @ 3 ms
Parallelizability	Good scalability up to 48 processors

Turbulence and scalar transport model(s)	RNG k-ε, Standard k-ε, LES-Smagorinsky
Spray models	Breakup: KH-RT with breakup length concept Collision model: NTC, O'Rourke Coalescence model: Post Collision outcomes Drag-law: Dynamic model
Time step	Variable based on spray, evaporation, combustion processes
Turbulence-chemistry interactions model	Direct Integration of detailed chemistry well-mixed (no sub-grid model)
Time discretization scheme	PISO (Pressure Implicit with Splitting of Operators)
Chemistry acceleration	Analytical Jacobian

Adaptive Mesh Generation



Base Grid Size = 4 mm, Minimum Grid Size = 0.5 mm

LES Turbulence Model

The density weighted LES spatial filtering operation on the Navier-Stokes equation results in the filtered momentum equation:

$$\frac{\partial \overline{\rho}\,\tilde{u}_i}{\partial t} + \frac{\partial \overline{\rho}\,\tilde{u}_i\,\tilde{u}_j}{\partial x_j} = -\frac{\partial \overline{P}}{\partial x_i} - \frac{\partial \overline{\rho} T_{ij}}{\partial x_j} + \frac{\partial}{\partial x_j}\left(\mu \frac{\partial \tilde{u}_i}{\partial x_j}\right) - \overline{F}_i$$

where the LES sub-grid scale tensor: $T_{ij} = \left(\tilde{u_i u_j} - \tilde{u}_i \tilde{u}_j\right)$

is modeled using a Smagorinsky based model: $T_{ij} = -2C_s\Delta^2\left|\overline{S}\right|\overline{S_{ij}} + \frac{1}{3}\delta_{ij}T_{kk}$

where $\left|\overline{S}\right| = \sqrt{2\overline{S_{ij}}\,\overline{S_{ij}}}$ $\quad \Delta = V_{cell}^{1/3}$ $\quad \overline{S_{ij}} = \frac{1}{2}\left(\frac{\partial \overline{u_i}}{\partial x_j} + \frac{\partial \overline{u_j}}{\partial x_i}\right)$

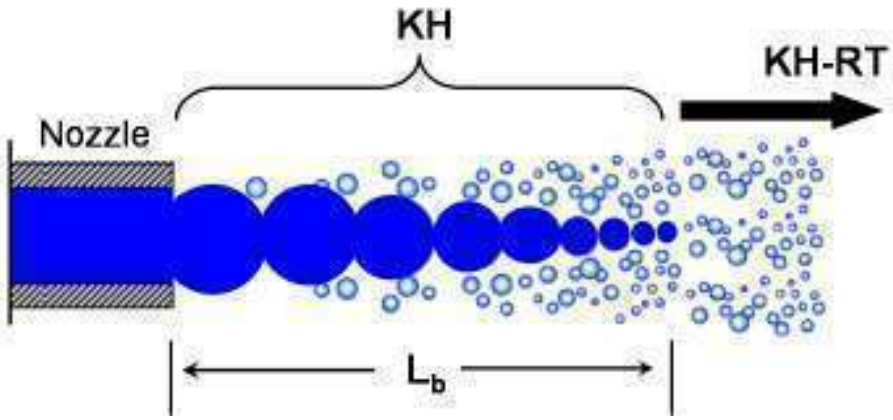
Sub-grid turbulent kinetic energy:

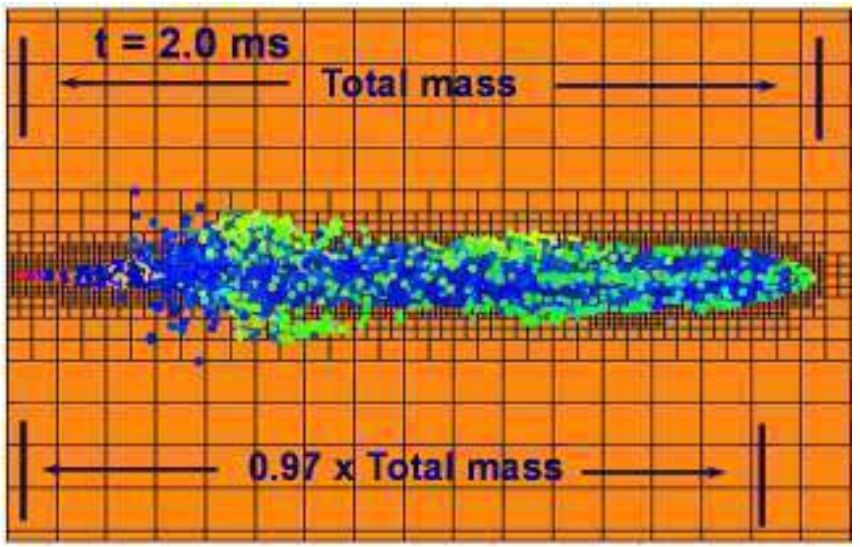
$$k \cong C_{les}\frac{\Delta^2}{24}\frac{\partial \overline{u_i}}{\partial x_j}\frac{\partial \overline{u_i}}{\partial x_j}$$

C_s = 0.2 **C_{les} = 2.0**

Definitions

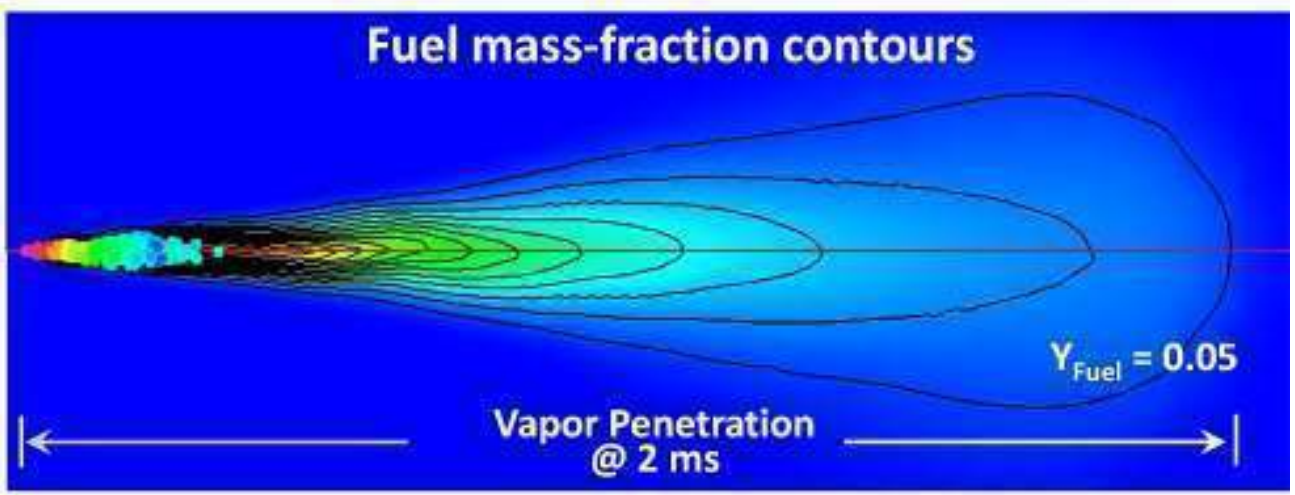
Break-up Length





Spray penetration @ 2 ms

Simulations with KH-ACT model not shown!

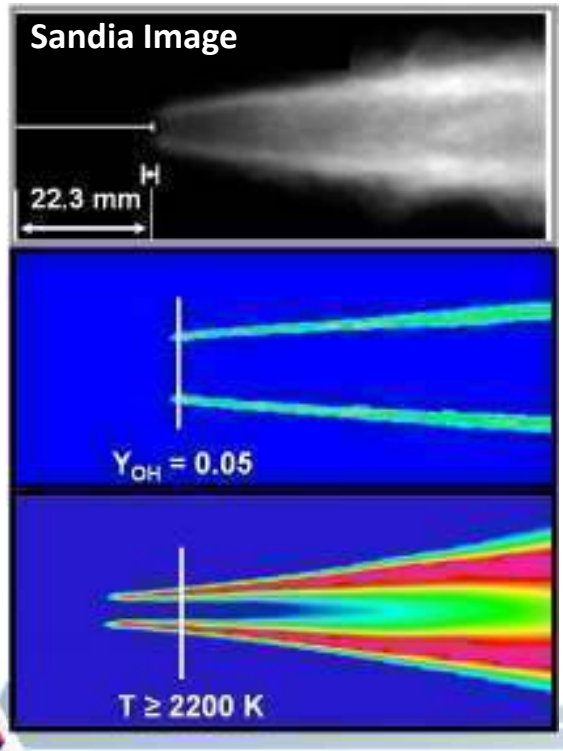


Spray and Combustion Set-up

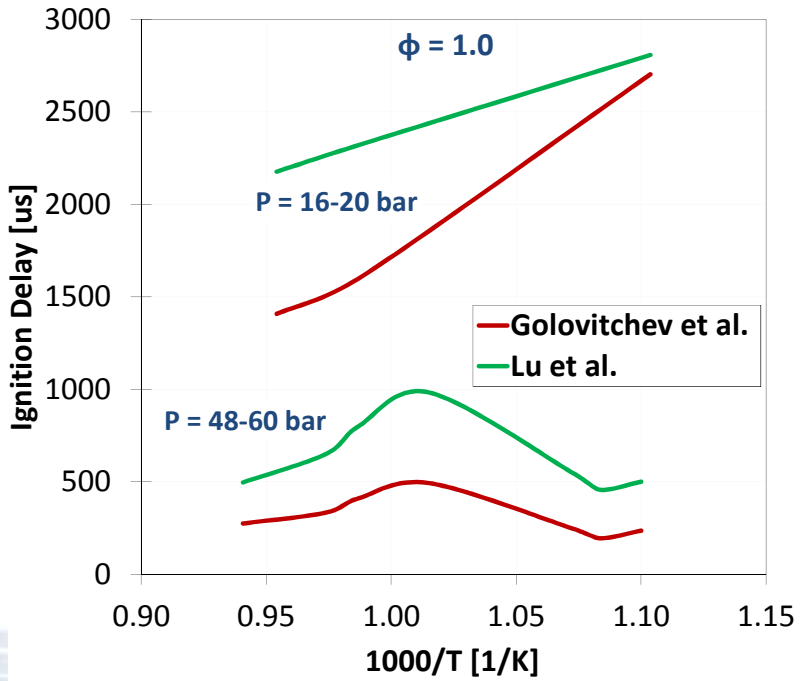
Chemical Kinetic Mechanism

1) 42 species, 283 reactions (**Golovitchev et al.**):
   V. I. Golovitchev, N. Nordin, R. Jarnicki, J. Chomiak. "3-D Diesel Spray Simulations Using a New Detailed Chemistry Turbulent Combustion Model," SAE Paper 2000-01-1891.
2) 68 species, 168 reactions (**Lu et al.**):
   Lu T. F., Law C.K., Yoo C.S., and Chen J.H., "Dynamic Stiffness Removal for Direct Numerical Simulations," Combustion and Flame, Vol. 156 No. 8 pp.1542-1551, 2009.

Lift-off length



Ignition delay: Ignition is said to occur when T ≥ 2000 K in a particular cell. Usually, coincides with appearance of OH.



Parametric Studies

- **Effect of turbulence model**
  - 1: RANS - Standard k-ε, RNG k-ε
  - 2: LES - Smagorinsky
- **Spray Structure**:
  - 1: Effect of grid-size: 0.5 mm, 1.0 mm, 2.0 mm
  - 2: Effect of time-step size

Non-reacting conditions for Spray A

- **Effect of Oxygen Concentration**:
  - 1: RANS-Golovitchev et al.(LOL, ID)
  - 2: RANS-Lu et al. (LOL, ID)
- **Effect of Ambient temperature**:
  - 1: RANS-Golovitchev et al. (LOL, ID)
  - 2: RANS-Lu et al. (LOL, ID)
  - 3: LES-Golovitchev et al. (LOL similar to RANS, Only ID)
- **Effect of Ambient density**:
  - 1: RANS-Golovitchev et al.(LOL, ID)
  - 2: RANS-Lu et al. (LOL, ID)

Reacting conditions for n-heptane

Note: Same set of spray constants were used for all parametric studies

(1) S. Som et al. , Combustion and Flame 2010
(2) S. Som, D.E. Longman & co-workers, ASME-ICE 2011

UW-ERC LES Spray Modeling

Prof. Chris Rutland

Nidheesh Bharadwaj

Noah Van Dam

Numerical setup and modeling approach

CFD code	KIVA 3V Release 2 (Amsden 1993)
Spatial disretization	2nd order (Amsden 1989)
Time integration	1st order (Amsden 1989)
Gas phase turbulence model	LES (dynamic structure model)
Droplet collision	O'Rourke (1981)
Spray breakup	Kelvin-Helmoltz Rayleigh-Taylor (KH-RT) model (Beale and Reitz 1999)
Turbulent dispersion	Gaussian (based on k_{sgs})

Turbulence modeling: *LES vs RANS*

Both RANS and LES

$$\frac{\partial \bar{\rho}\langle u_i\rangle}{\partial t}+\frac{\partial \bar{\rho}\langle u_i\rangle\langle u_j\rangle}{\partial x_j}=-\frac{\partial \bar{p}}{\partial x_i}+\frac{\partial \overline{\tau_{ij}^{m}}}{\partial x_j}-\frac{\partial \langle \rho\rangle \Gamma_{ij}}{\partial x_j}$$

$$\left.\begin{array}{l}\text{Sub-grid shear stress (LES)}\\ \text{Reynolds Stress (RANS)}\end{array}\right\}=\Gamma_{ij}=\begin{cases} c_{ij}\,2k & \text{..... LES (DSM)} \\ \underbrace{(ck^2/\varepsilon)}_{\nu_T}\dfrac{\partial u_i}{\partial x_j} & \text{..... RANS (RNG)}\end{cases}$$

k^{sgs}

TKE *(Turbulent KE)*

Diffusion Dissipation Production Spray Source

$$\frac{\partial(\bar{\rho}k_{sgs})}{\partial t}+\frac{\partial(\bar{\rho}\langle u_j\rangle k_{sgs})}{\partial x_j}=\underbrace{D}_{=-\frac{\partial}{\partial x_j}(\mu_T\frac{\partial k}{\partial x_j})}-\underbrace{\varepsilon}_{=C_1\rho\frac{k^{3/2}}{\Delta}}+\underbrace{P}_{=\langle u_i\rangle\frac{\partial \rho\overline{\Gamma}_{ij}}{\partial x_j}}+\dot{W}_s$$

Focus on spray source modeling in LES context

Spray source/sink term model

$$\dot{W}_s = -\underbrace{\left(u_i(\vec{x}_d,t) - \langle u_i \rangle\right)}_{u_i^{slip}} \underbrace{\iint_S G(\vec{x}-\vec{\zeta})\left\{\sigma_{ij}(\vec{\zeta},t) - \bar{\sigma}_{ij}(\vec{x},t)\right\} dA_j}_{F_i} = -F_i u_i^{sgs}$$

Drag from the gas to the drop

SGS gas velocity (obtained using de-convolution)

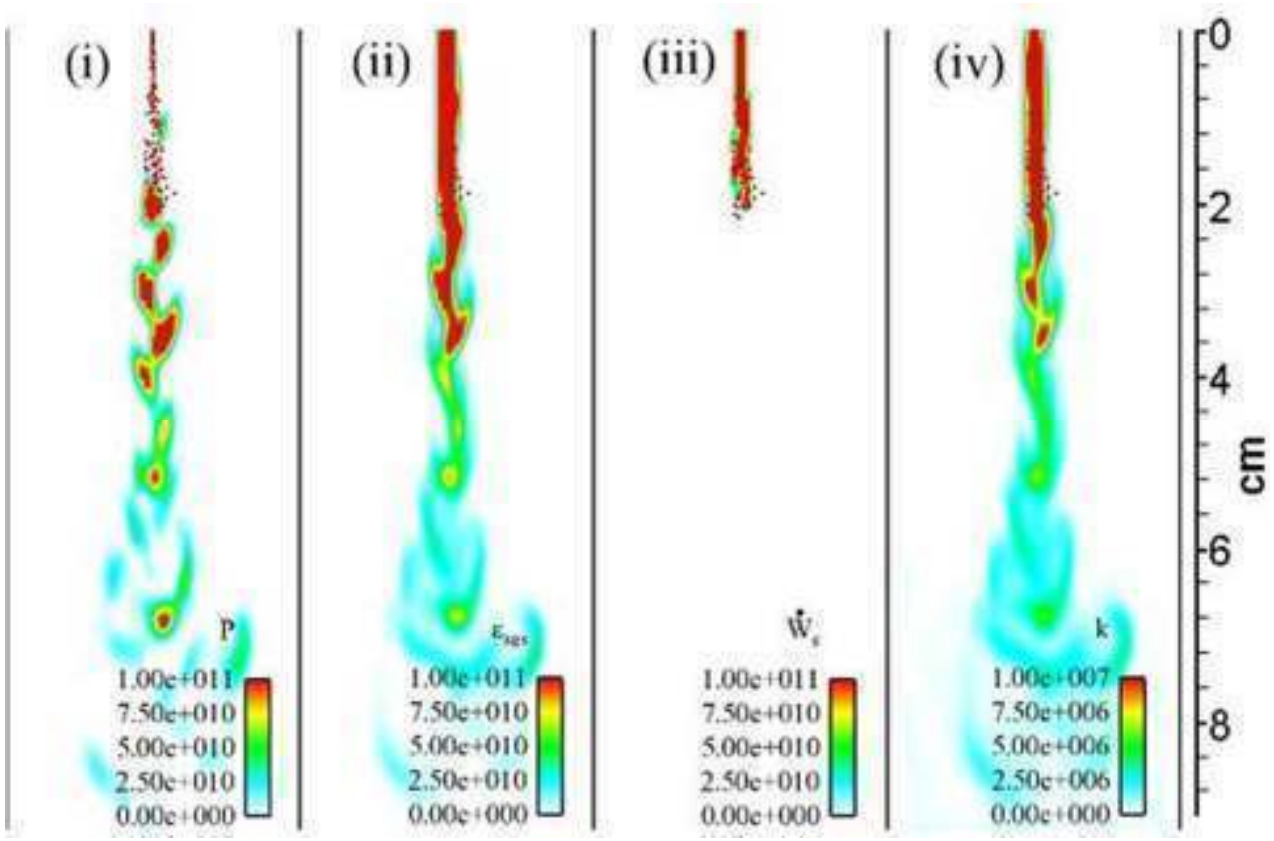
- Drag (F) based on resolved velocity field [standard KIVA model]
- Sub-grid velocity from Approximate Deconvolution Method (ADM) [Stolz & Adams 1999]

$$\dot{W}_s = -\frac{3}{8}\frac{C_d}{V_{cell}} \sum_d \left\{ \underbrace{\frac{m_d \bar{\rho}\, V_{rel}}{r_d \bar{\rho}_l}\left(\langle u_i \rangle + u'_{p,i} - u_{d,i}\right)}_{F_i} \underbrace{\left(2\langle u_i \rangle - 3\langle\langle u_i \rangle\rangle + \langle\langle\langle u_i \rangle\rangle\rangle\right)}_{u_i^{sgs}} \right\}$$

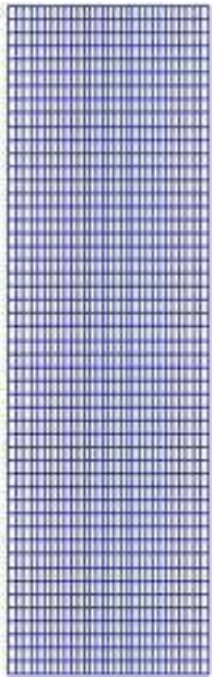
Final form

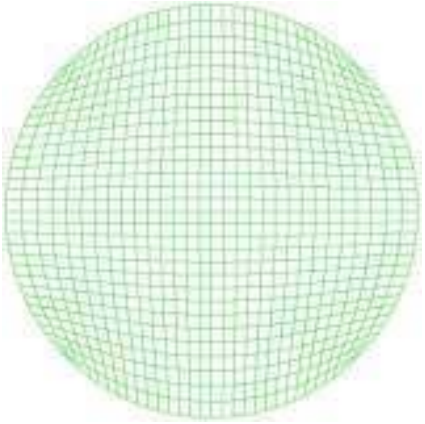
Important terms in k_{sgs} transport equation

Production | Dissipation | Spray source term | k_{sgs}: sub-grid kinetic energy



Spray A Mesh Configuration

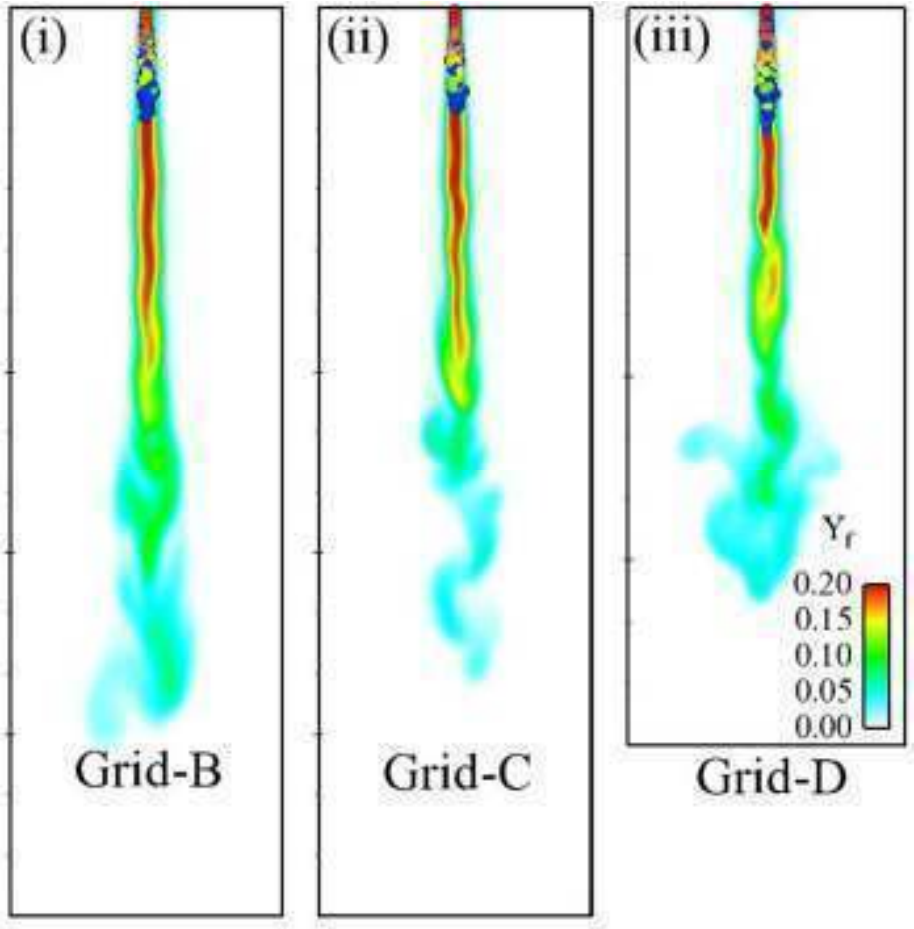


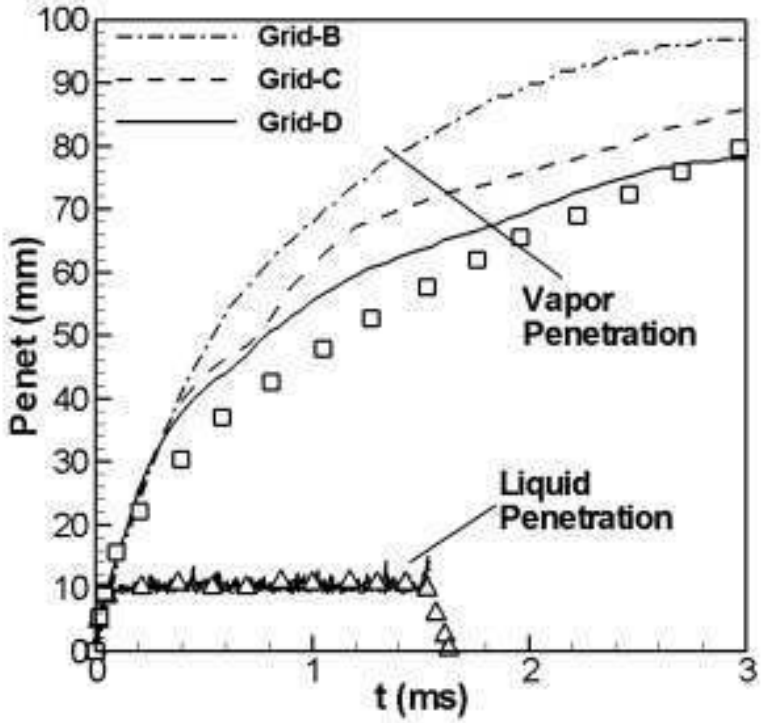


Grid specification

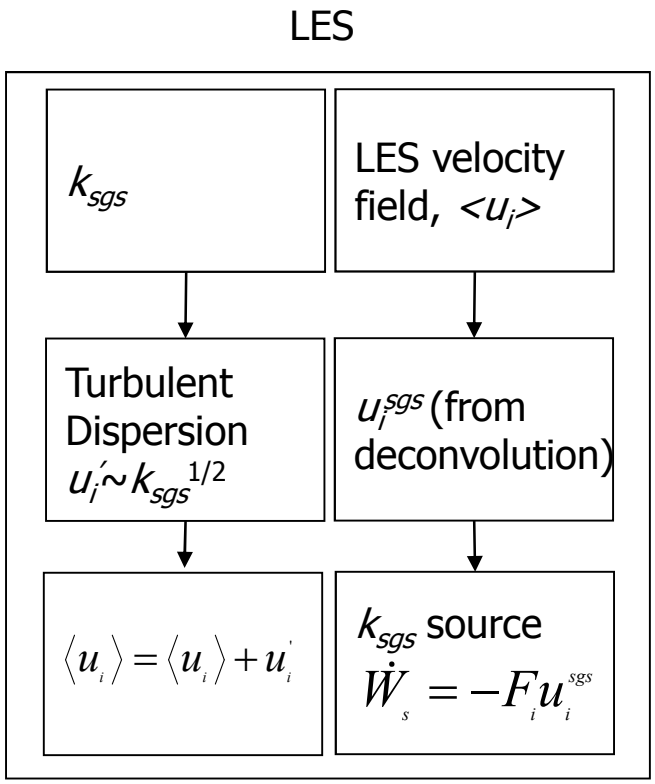
	dx (mm)	dy (mm)	dz (mm)
Grid-A	1	1	1
Grid-B	0.5	0.5	1
Grid-C	0.5	0.5	0.67
Grid-D	0.5	0.5	0.5

Comparison with recent "Spray-A" measurements at Sandia National Lab





LES Model Implementation in KIVA code



- Where u_i' is the random fluctuating velocity obtained using a Gaussian PDF

Turbulence modeling: *LES vs RANS*

Both RANS and LES

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k^{sgs}

TKE *(Turbulent KE)*

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Final form

ECN spray modeling at Politecnico di Milano

G. D'Errico, T. Lucchini

Internal Combustion Engine Group
Department of Energy
Politecnico di Milano

Politecnico di Milano

POLITECNICO DI MILANO

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Temporary Researchers

Daniele Ettorre, MSc
Marco Fiocco, MSc

Ph.D students

Andrea Montorfano, MSc
Augusto Della Torre, MSc

Post-doc researchers

Tarcisio Cerri, PhD

MSc students

15-20 per year

PoliMI method and results

POLITECNICO DI MILANO

CODE

OpenFOAM® with libraries and solvers for internal combustion engine developed at Politecnico di Milano (Lib-ICE package).

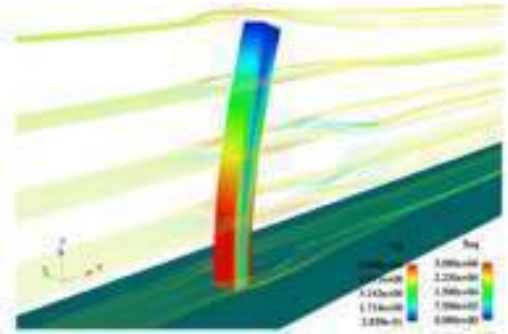
OpenFOAM is a free-to-use Open Source numerical simulation software with extensive CFD and multi-physics capabilities, written in a highly efficient C++ object-oriented programming.

Impressive diffusion with 2000 downloads/ week.

Very extended physical modelling capabilities

Ideal platform for research collaborations.

Physics model implementation through **equation mimicking**. Possibility of extension to non-traditional, complex or coupled physics.



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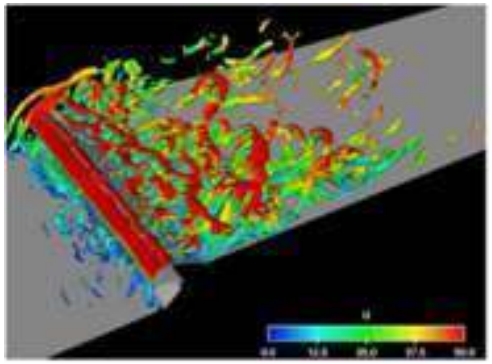
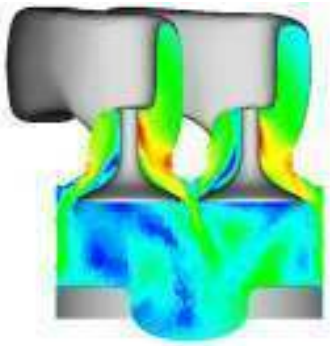


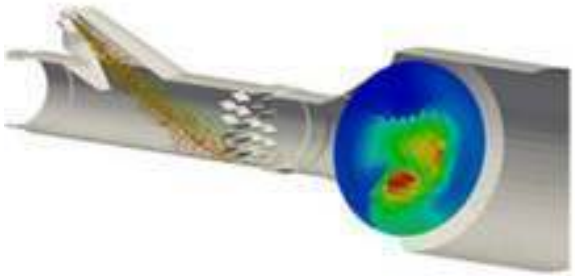
PoliMI method and results

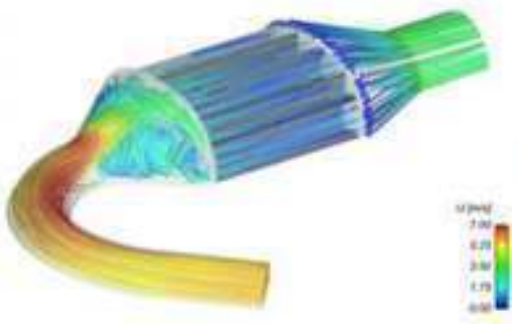
POLITECNICO DI MILANO

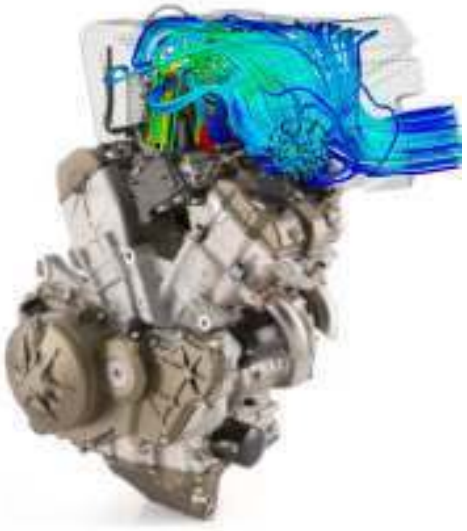
The ICE group of Politecnico di Milano has contributed to develop the engine library under **OpenFOAM** technology (**Lib-ICE**):

- Moving mesh algorithms
- Spray modeling
- Combustion process modeling
- 1D-3D coupling interface
- Non-linear acoustics modeling
- DPF and SCR modeling







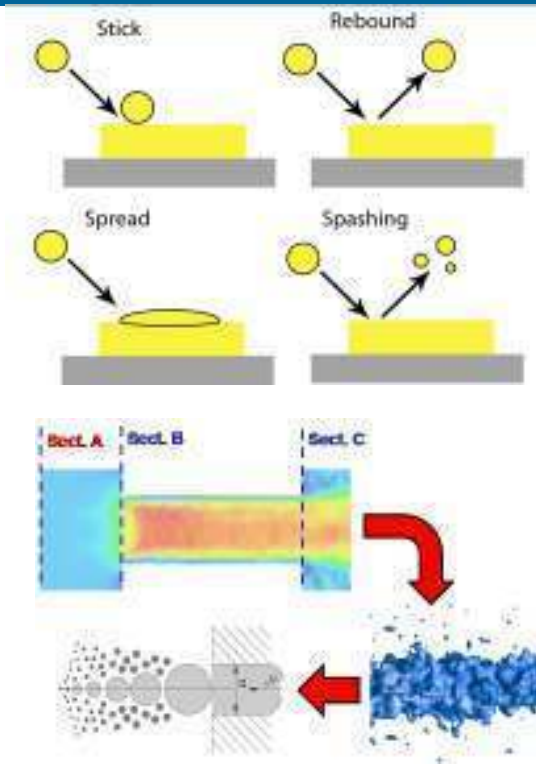


Spray models

POLITECNICO DI MILANO

Implemented capabilities:

Injection	**Blob, Huh, Hollow-cone, Pressure-Swirl**
Atomization	**Huh-Gosman, Bianchi, WAVE, LISA**
Breakup	**TAB, ETAB, KH-RT, Reitz-Diwakar**
Evaporation	**Frossling**
Heat-transfer	**Ranz-Marschall**
Wall impingement	**Stanton, Naber-Reitz, Bai-Gosman**
Collision	**Nordin, O'Rourke**



- Development of new **atomization** models (**Huh-Gosman** and **Bianchi**) to describe liquid-jet atomization of high pressure liquid jets. Model tuning constants derived from multi-phase LES simulations of liquid jet breakup.
- Development of **droplet-wall interaction** and **liquid film** models to correctly account for the influence of wall impingement on combustion and fuel-air mixing processes.

PoliMI results

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ECN contribution

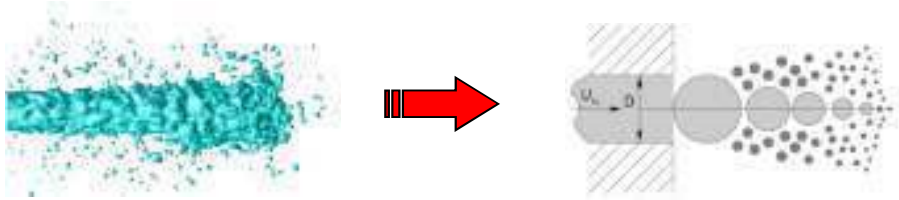
Simulation of Baseline and SprayA test cases

SPRAY MODEL CHOICE

Discrete Droplet Model (DDM)

Bianchi model for injection and atomization. It is a modified version of the Huh-Gosman model where multiphase LES calculations were used to tune the main model coefficients (C_1,..,C_5, C_w) and to compute secondary droplet diameter.

Turbulent quantities (L_t, t_t) initialized for each parcel according to the nozzle flow conditions.



Wave model (based on Kelvin-Helmholtz theory) for secondary breakup

Other models: Frossling for evaporation, Ranz-Marschall for heat-transfer, turbulent dispersion (stochastic). Collision was not taken into account.

Modified Huh-Gosman model

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- Diameter reduction of the injected parcels:

$$\frac{dD}{dt} = -C_5 \frac{L_a}{\tau_a} \Rightarrow \begin{cases} L_a = C_2 \cdot L_t \\ \tau_a = C_1 \cdot \tau_t + C_4 \cdot \tau_w \end{cases}$$

- L_t: turbulent length-scale, supposed to be constant.
- t_t: turbulent time-scale ($t_t = t_{t0} + 0.1 \cdot t$).
- t_w: wave-growth time-scale (Kelvin-Helmholtz).

C_1	C_2	C_4	C_5
2.0	0.5	0.3	0.7

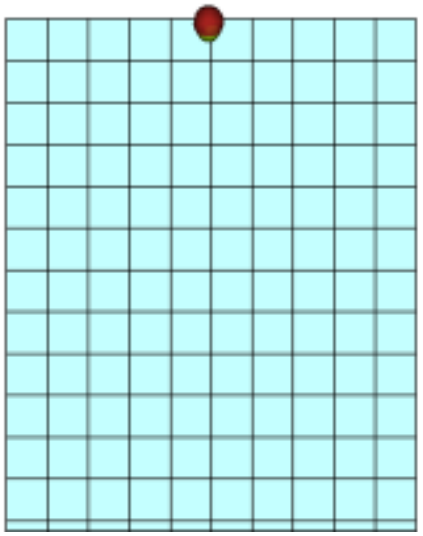
No tuning or parameterization was performed:
same constants for Baseline nheptane and SprayA case

PoliMI method and results

POLITECNICO DI MILANO

NUMERICAL TECHNIQUES

Adaptive Local Mesh Refinement (ALMR)



Total fuel mass in one cell is the error estimator: Y_{l+g}

Grid refined when: $Y_{\min} \leq Y_{l+g} \leq Y_{\max}$

Arbitrary level of refinements allowed.

Works with hexahedral topology and moving meshes.

Direct integration of detailed chemistry (DICC)

Each cell is considered to be perfectly mixed

No turbulence-chemistry interaction

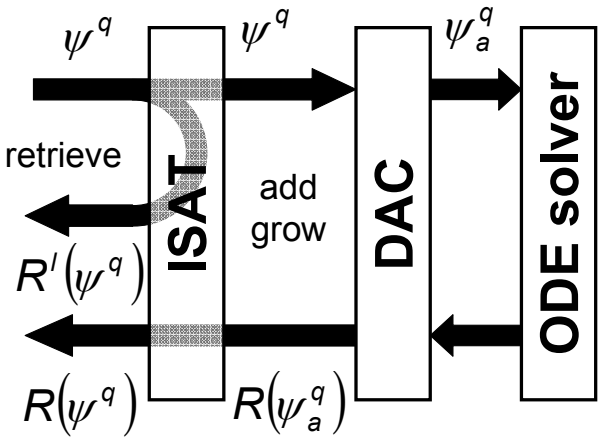
ODE stiff solver (semi-implicit Burlish-Stoer, SIBS)

TDAC algorithm

Tabulation of Dynamic Adaptive Chemistry

It combines ISAT (in-situ adaptive tabulation) and DAC (dynamic adaptive chemistry).

CPU speed up factors from 50-500.



PoliMI method and results

POLITECNICO DI MILANO

PoliMI Best configuration set-up and legend for the parameter studies

PoliMI best set-up	
atomization:	Bianchi (modified Huh-Gosman)
breakup:	Kelvin-Helmholtz
turbulence:	Realizable k-epsilon
time step:	5.00E-07
mesh size	ALMR with minimum mesh size equal to 1 mm
chemistry	TDAC with scheme from Lu

Legend for the parameter studies

1	Best	
2	ALMR: min Mesh 0.5 mm	
3	ALMR: min Mesh 1.0 mm	best
4	ALMR: min Mesh 2.0 mm	
5	ALMR: min Mesh 4.0 mm	
6	time step: 5.e-6	
7	time step: 1.e-6	
8	time step: 5.e-7	best
9	time step: 1.e-7	
10	turbulence model: standard k-epsilon	
11	turbulence model: realizable k-epsilon	best
12	turbulence model: RNG k-epsilon	
13	DI of complex chemistry: scheme from Lu (56s)	best
14	DI of complex chemistry: scheme from Curran (159s)	
15	DI of complex chemistry: scheme from Patel (32s)	

Acknowlegments

The Diesel spray modelling activity at PoliMI is currently funded by:

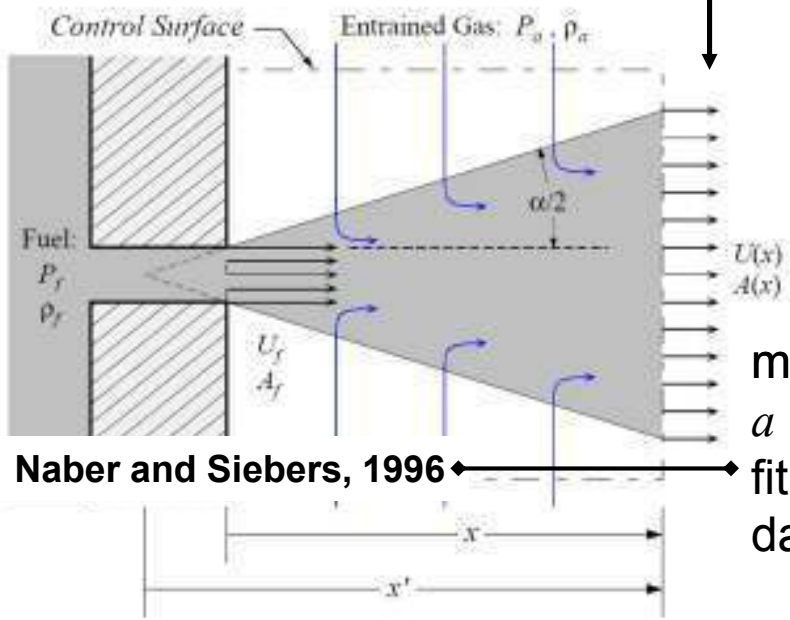
MAGNETI MARELLI

LIEBHERR

SEATEK

Evolution of analytical models to describe penetration and fuel-ambient mixing.

(1) Uniform Profile



Naber and Siebers, 1996

Mixing

$$\frac{F}{A} = \frac{2}{\sqrt{1+16\cdot\tilde{x}^2}-1}$$

$$\tilde{x} = x'/x^+ \qquad \tilde{\rho} = \rho_f/\rho_a$$

$$x^+ = \tilde{\rho}^{1/2}\left(\frac{\tilde{\rho}-m}{\tilde{\rho}}\right)\frac{\sqrt{C_a}\cdot d_0}{a\cdot\tan(\theta/2)}$$

model constant a = 0.66 when fit to penetration data

$$a\cdot\tan(\theta/2) = \tan(\alpha/2)$$

Smaller model angle

experimental spreading angle

Penetration

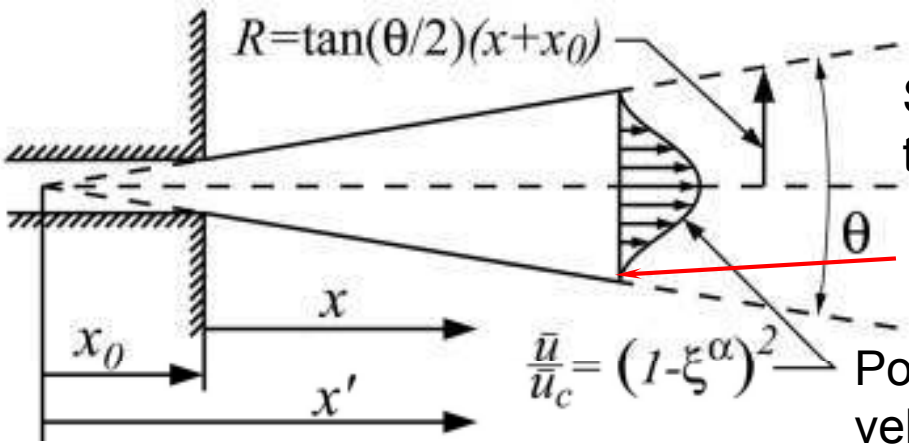
$$\tilde{S} = \tilde{x} = x'/x^+$$

$$\tilde{t} = \frac{\tilde{S}}{2} + \frac{\tilde{S}}{4}\cdot\sqrt{1+16\cdot\tilde{S}^2} + \frac{1}{16}\cdot\ln\left(4\cdot\tilde{S}+\sqrt{1+16\cdot\tilde{S}^2}\right)$$

- Used to estimate ambient entrainment, momentum transfer, penetration.
- Mixing estimate also used for vaporization and combustion analysis:
  - Liquid length (Siebers, 1999)
  - Lift-off length (Siebers and Higgins, 2001)

Evolution of analytical models to describe penetration and fuel-ambient mixing.

(2) Variable Profile



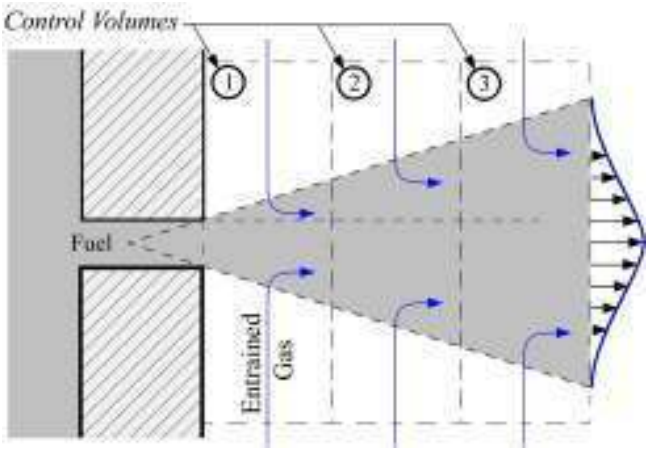
Musculus and Kattke, 2009

Spreading angle still required as input to the model.

Z = 0 (for FWHM, s.a. is ≈ 45% of this angle).

Polynomial profile (used for fuel mass and velocity) resembles a Gaussian radial distribution.

- Variable-profile model also based on momentum and mass transfer.
- Analytical solution for mixing and penetration exists if steady injection rate.
  - For variable rate of injection, or after the end of injection, Musculus and Kattke use multiple, discrete control volumes.



Engine Combustion Network (n-heptane and Spray A) Modeling

Y. Pei, E. R. Hawkes and S. Kook
Engine Research Group
The University of New South Wales
May 13th, 2011

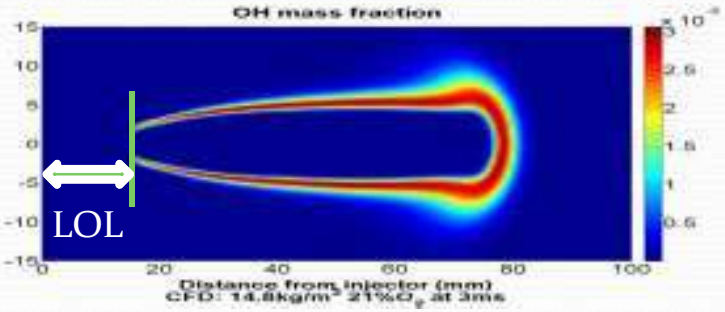
THE UNIVERSITY OF NEW SOUTH WALES

SYDNEY · AUSTRALIA

Spray and Combustion Setup

	n-heptane	Spray A
Code	Fluent 13.0	
Turbulence model	Realizable k-ε	
Spray model	Discrete Phase Model with "Blob" method, Stochastic DRW, Ranz-Marshall, Sherwood number correlation	
Drag law	Stokes-Cunningham /High-Mach-Number drag	Stokes-Cunningham drag
Second breakup model	"Wave" breakup , B1=14.5	"Wave" breakup , B1=22
Collision model	O'Rourke method	
Grid	Structured 2D axisymmetric	
Grid size	0.125mm to 0.5mm 100800 cells 0.25mm to 1mm 25200 cells 0.5mm to 2mm 6300 cells	0.25mm to 1mm 25200 cells
Spatial discretization	Second order upwind	
Turbulence-chemistry interactions	well-mixed	
Chemistry mechanism	Baseline ERC mech. SAE Paper 2004-01-0558	N/A
Chemistry acceleration	ISAT	N/A
Time discretization	PISO (Pressure-Implicit with Splitting of Operators)	
Time step size	1e-07s	

Definitions and parameter studies



Parameter studied	Definition
Liquid length	The axial position of leading particle
Vapor penetration length	The distance from the injector to 0.5% fuel vapor mass fraction layer
Lift-off length	The length from the injector to the closest layer where OH mass fraction reaches 0.02%
Ignition delay	The time from start of injection to the time where the maximum temperature of the domain is 400k above the initial ambient temperature

- Non-reacting case

  (spray structure)

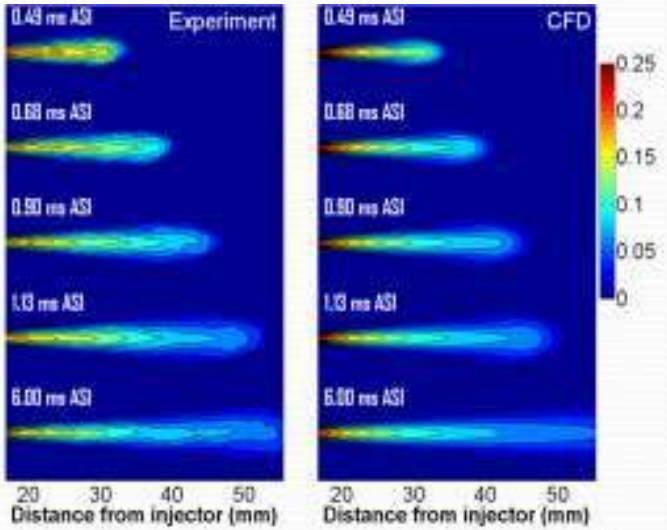
  - Mesh resolution
  - Time step size
  - Drag law

- Reacting case

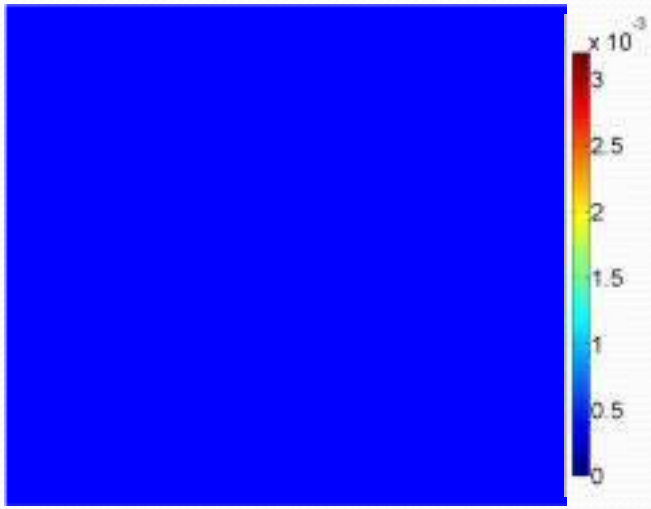
  (lift-off length and ignition delay)

  - Ambient O2 %
  - Initial ambient temperature
  - Ambient density

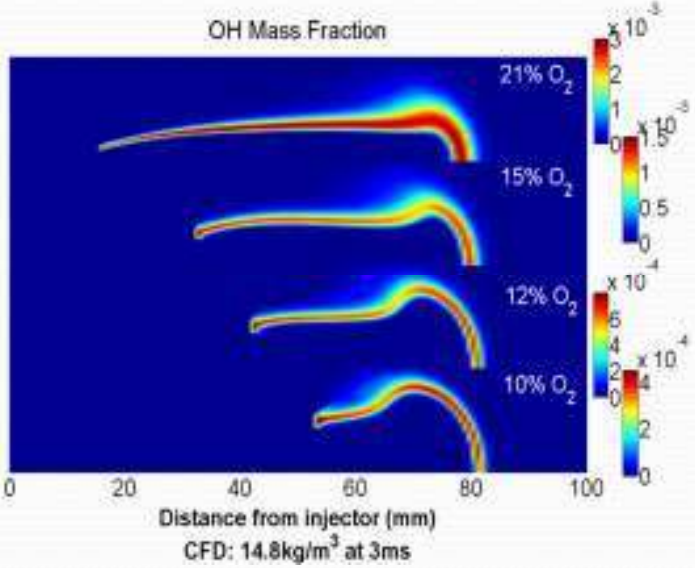
Plots and Animation

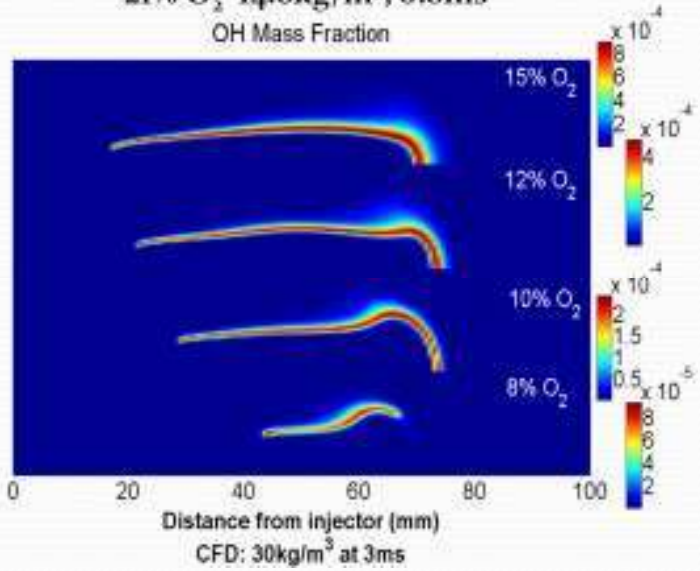


Temporal evolution of fuel mass fraction



OH temporal evolution
21% O_2 14.8kg/m³, 6.8ms





Compilation of Spray A Modeling Efforts

May 13th 2011

Sibendu Som

Argonne National Laboratory

Engine Combustion Network (ECN) Workshop 2011

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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!

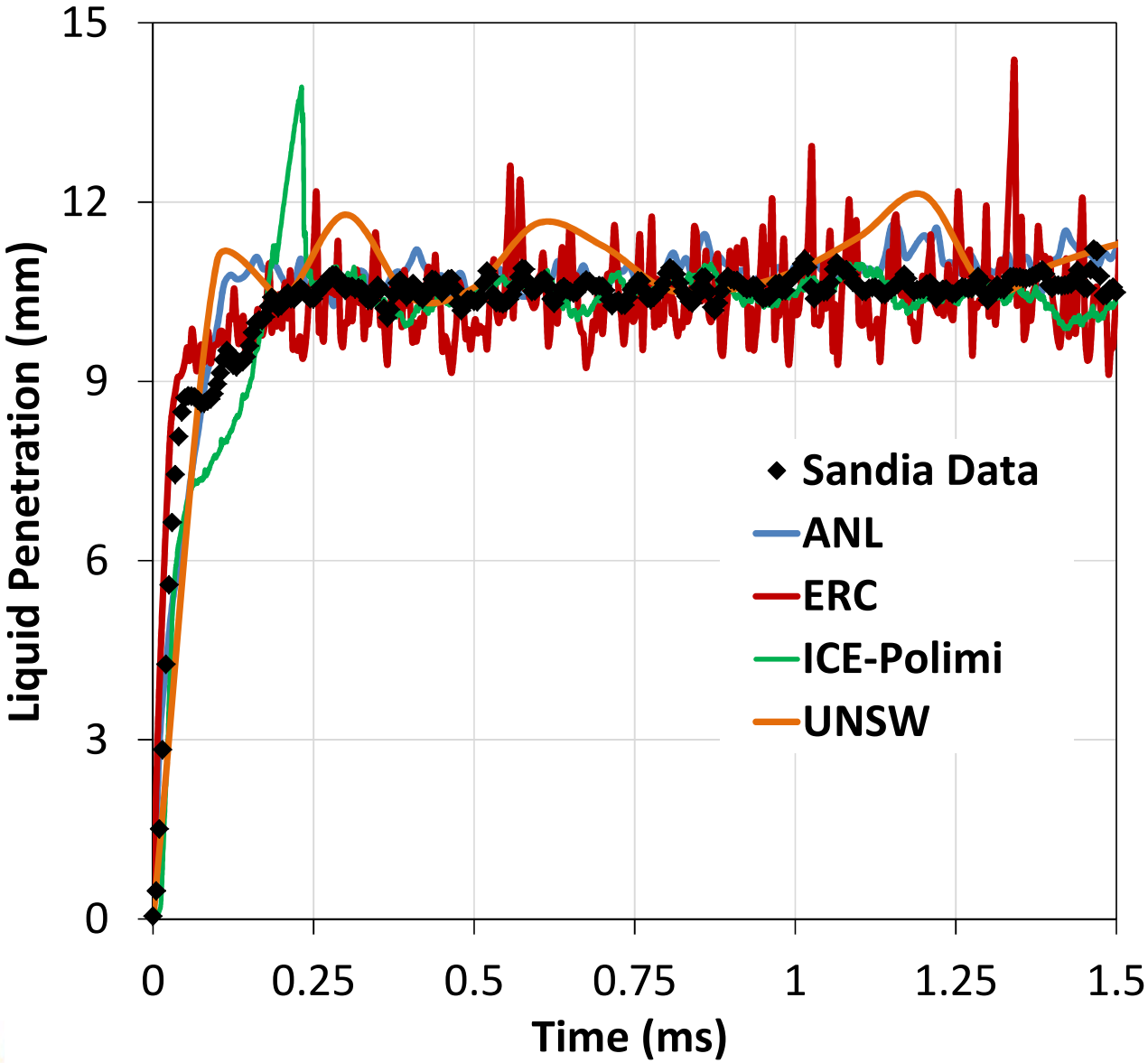
Baseline Spray A: non-reacting conditions

Parameter	Quantity
Fuel	N-dodecane (n-C12H26)
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

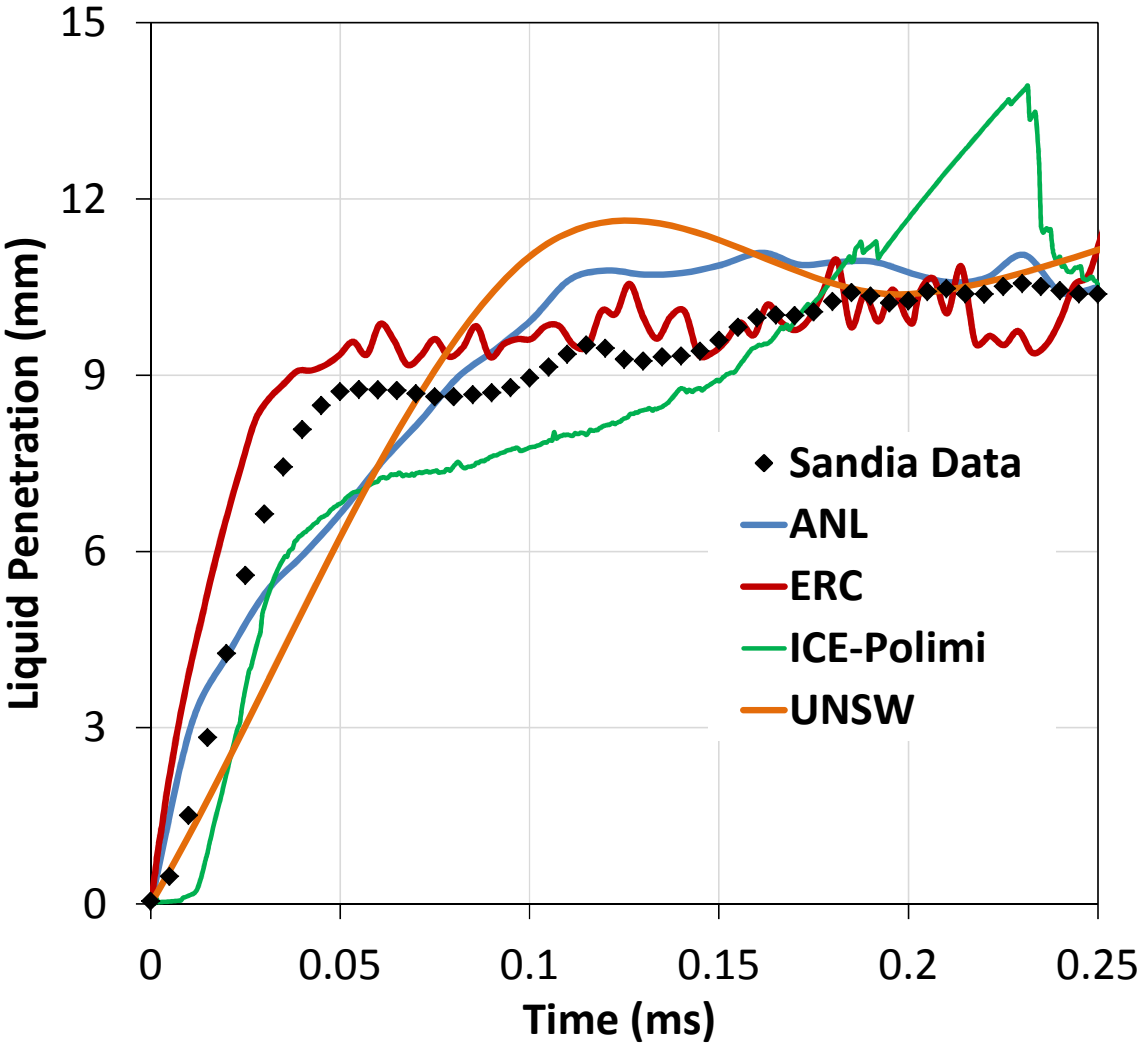
Spray Penetration vs. Time



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

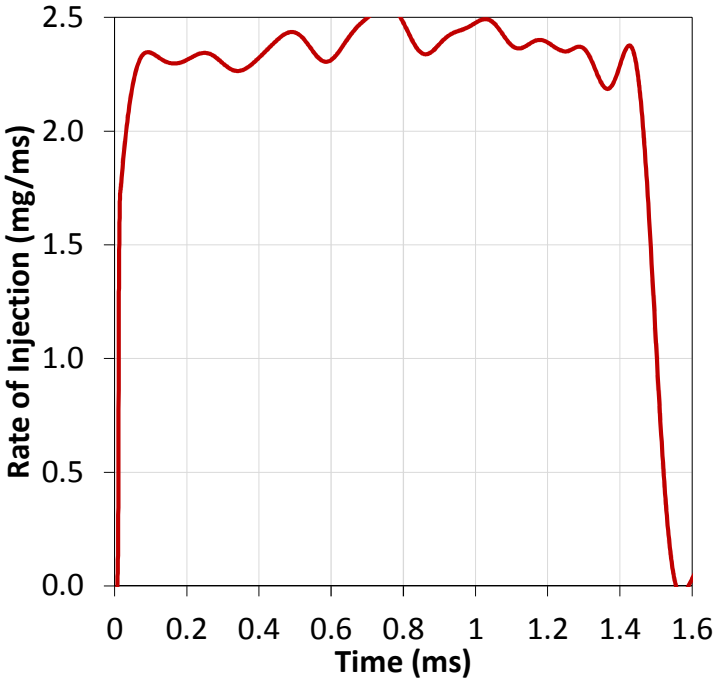
Liquid length fluctuations can be reduced by injecting higher number of computational parcels

Spray Penetration vs. Time

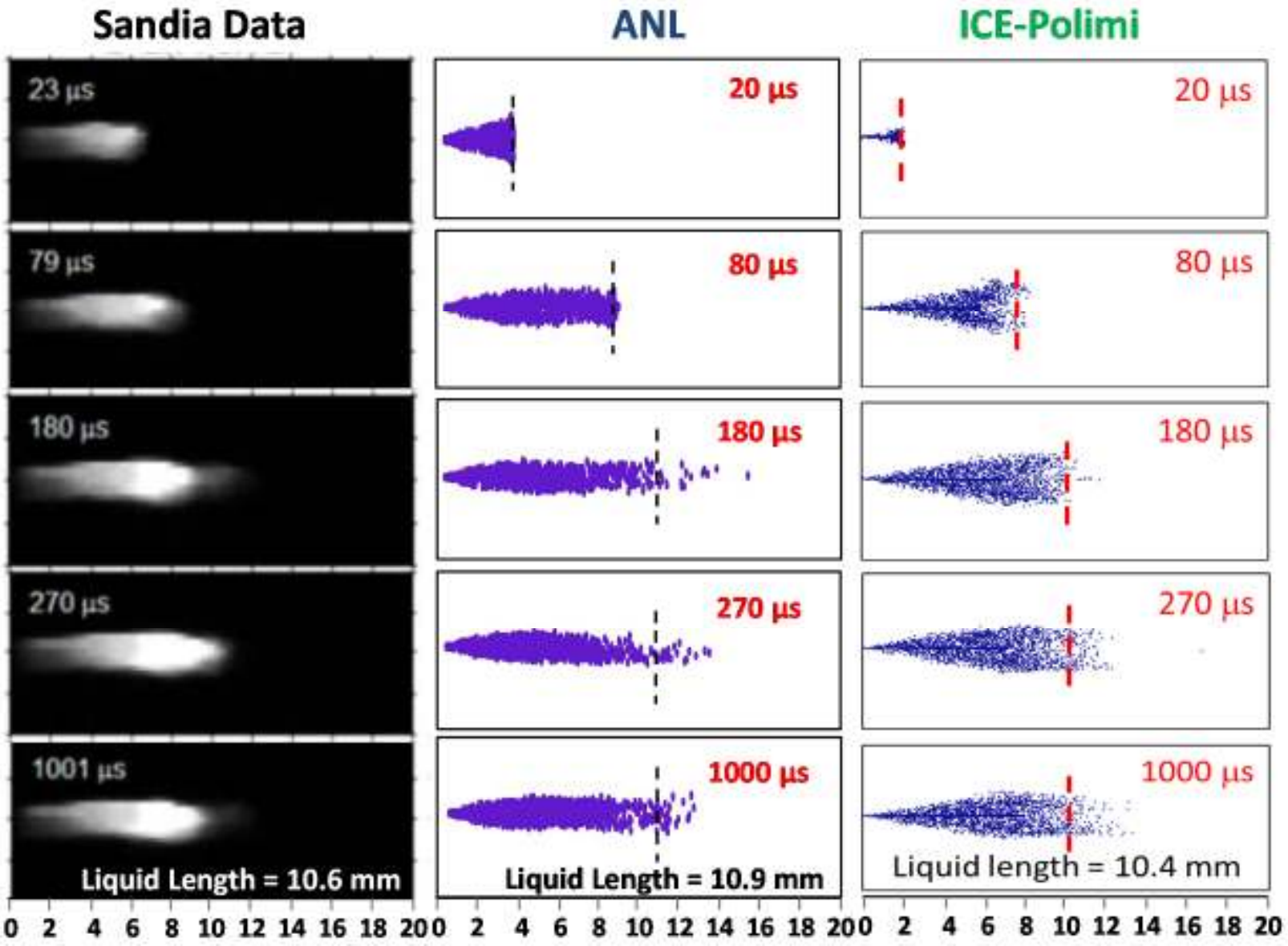


Initial transience not well predicted by any model. Possible causes:

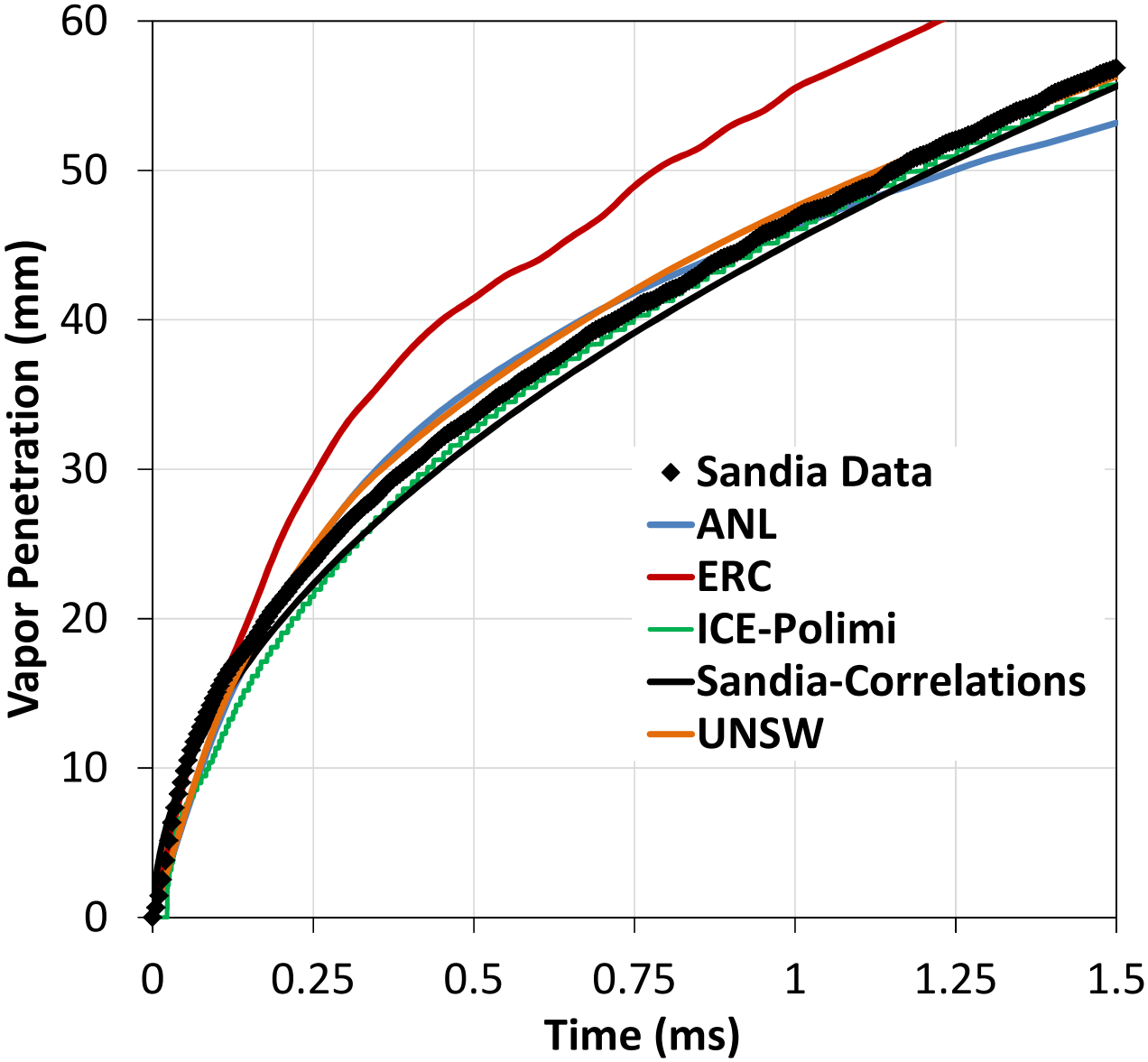
- Accurate representation of ROI?
- Need to account for nozzle geometry and needle-lift effects?

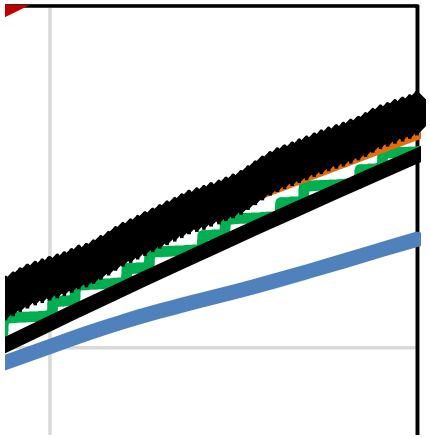


Liquid Spray Structure

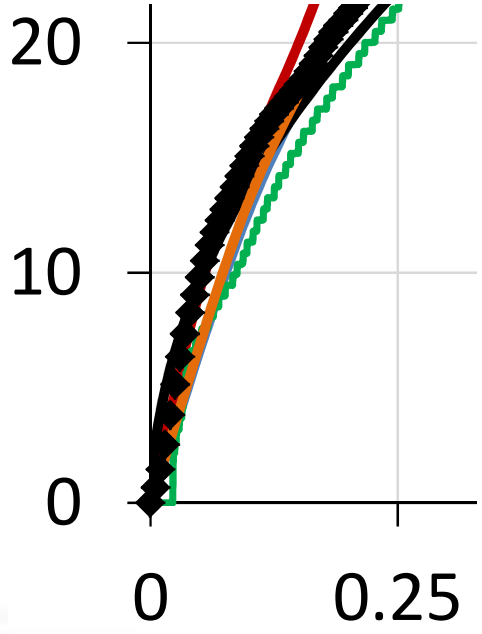


Vapor Penetration vs. Time

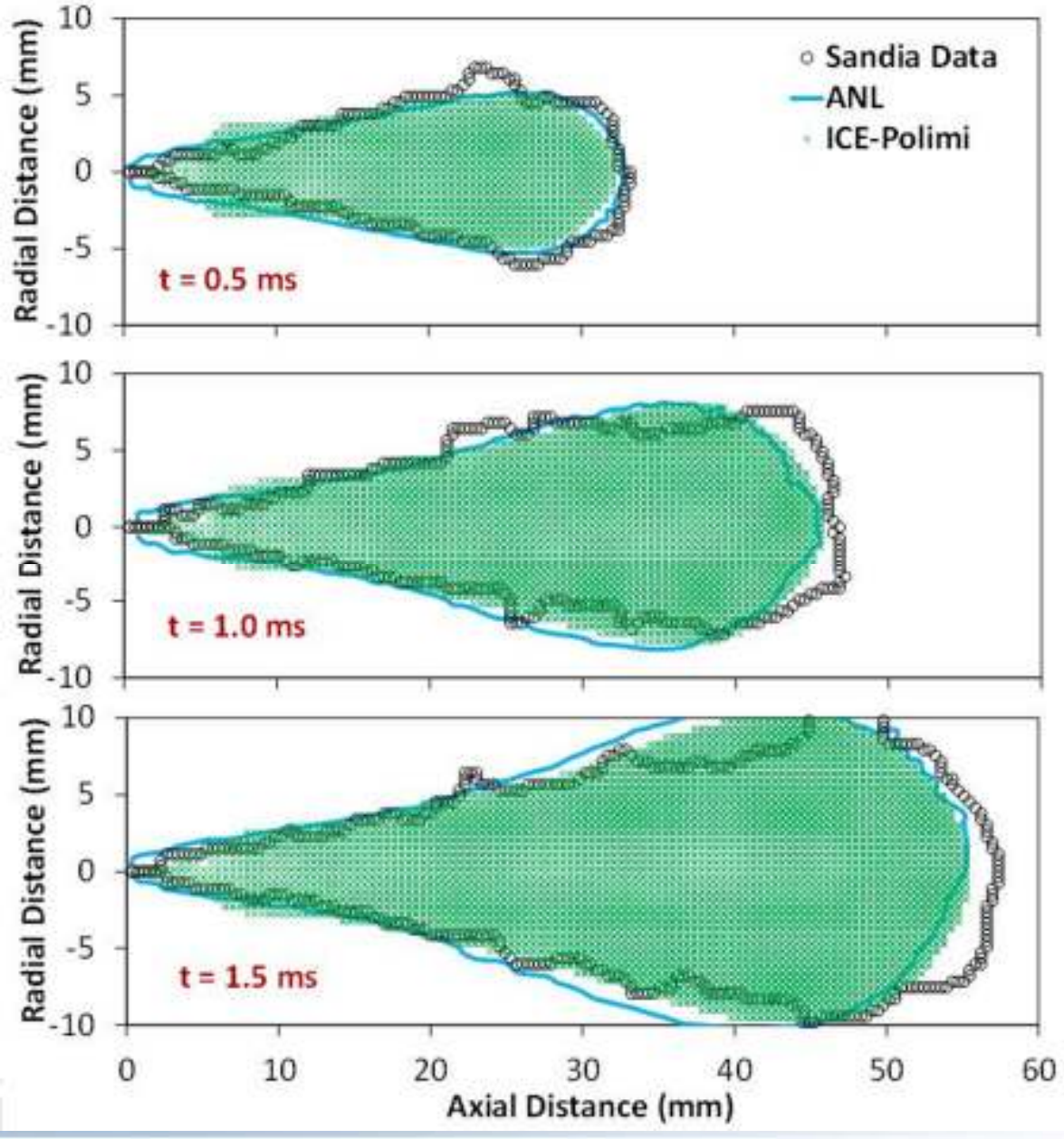




In general, the CFD models are unable to match the slopes



Vapor Boundary Comparison

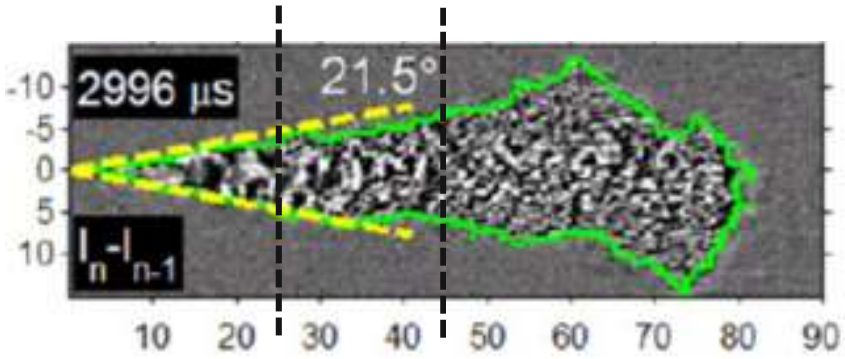


After 1.0 ms it is clear that the simulations are under-predicting vapor penetration

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

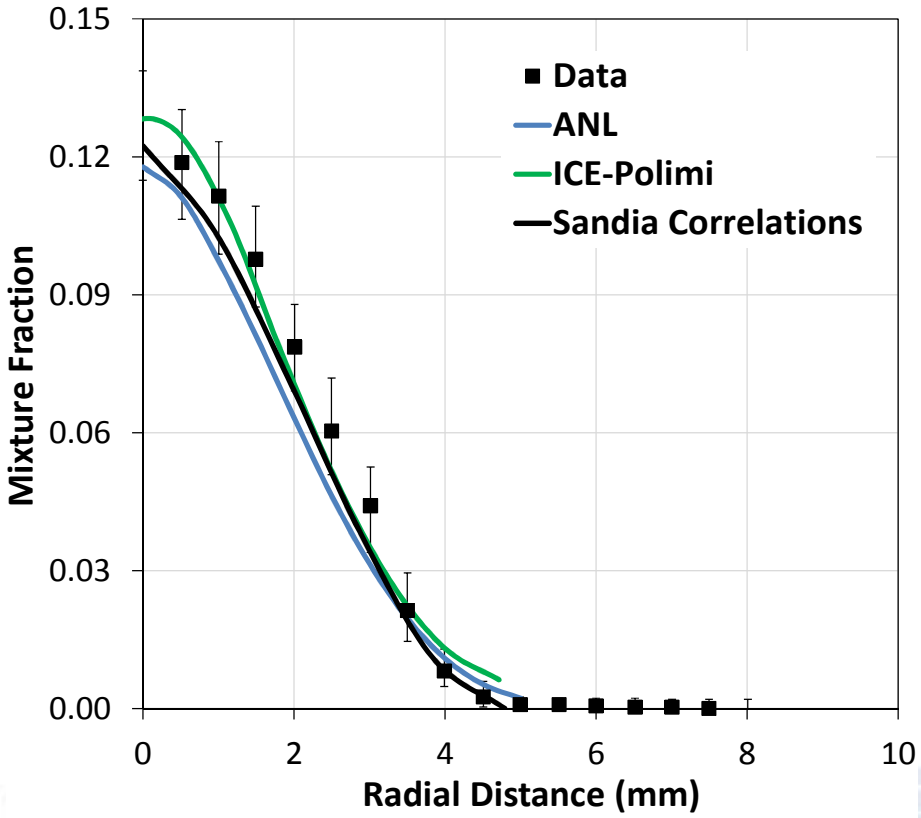
Probably a LES model can better predict the instantaneous structure of the spray

Radial Mixture fraction Distribution

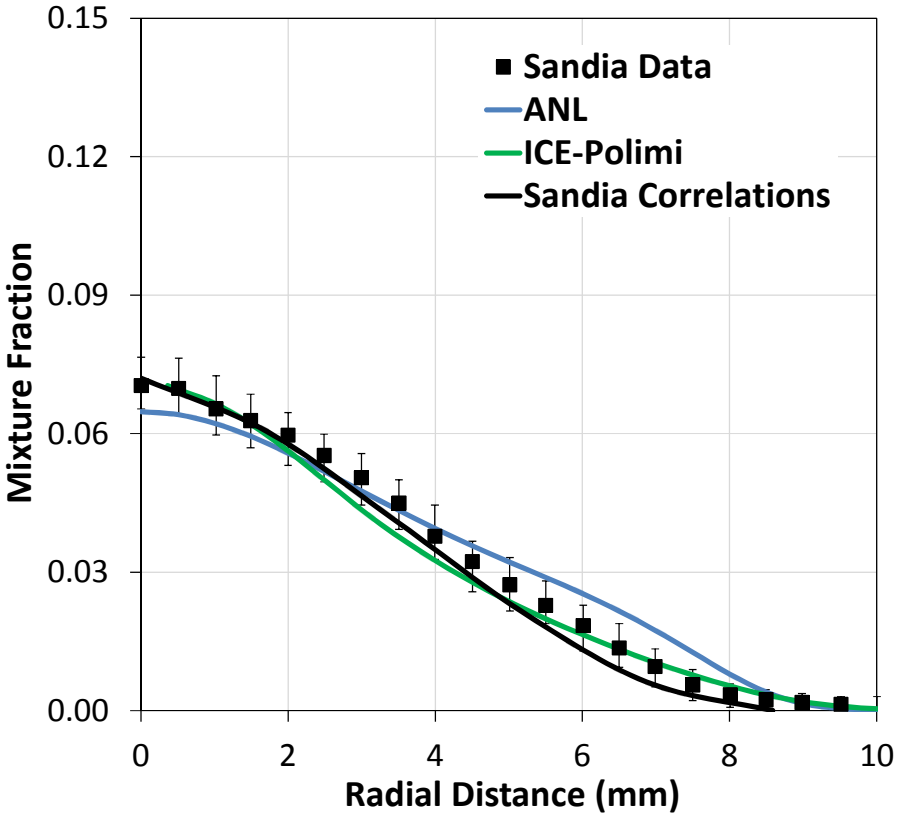


- Simulations plots at 1.5 ms
- In general, Gaussian mixture fraction profiles are well-predicted by all models at both axial locations
- Mixture fraction distribution along the center line need to be compared

X = 25 mm

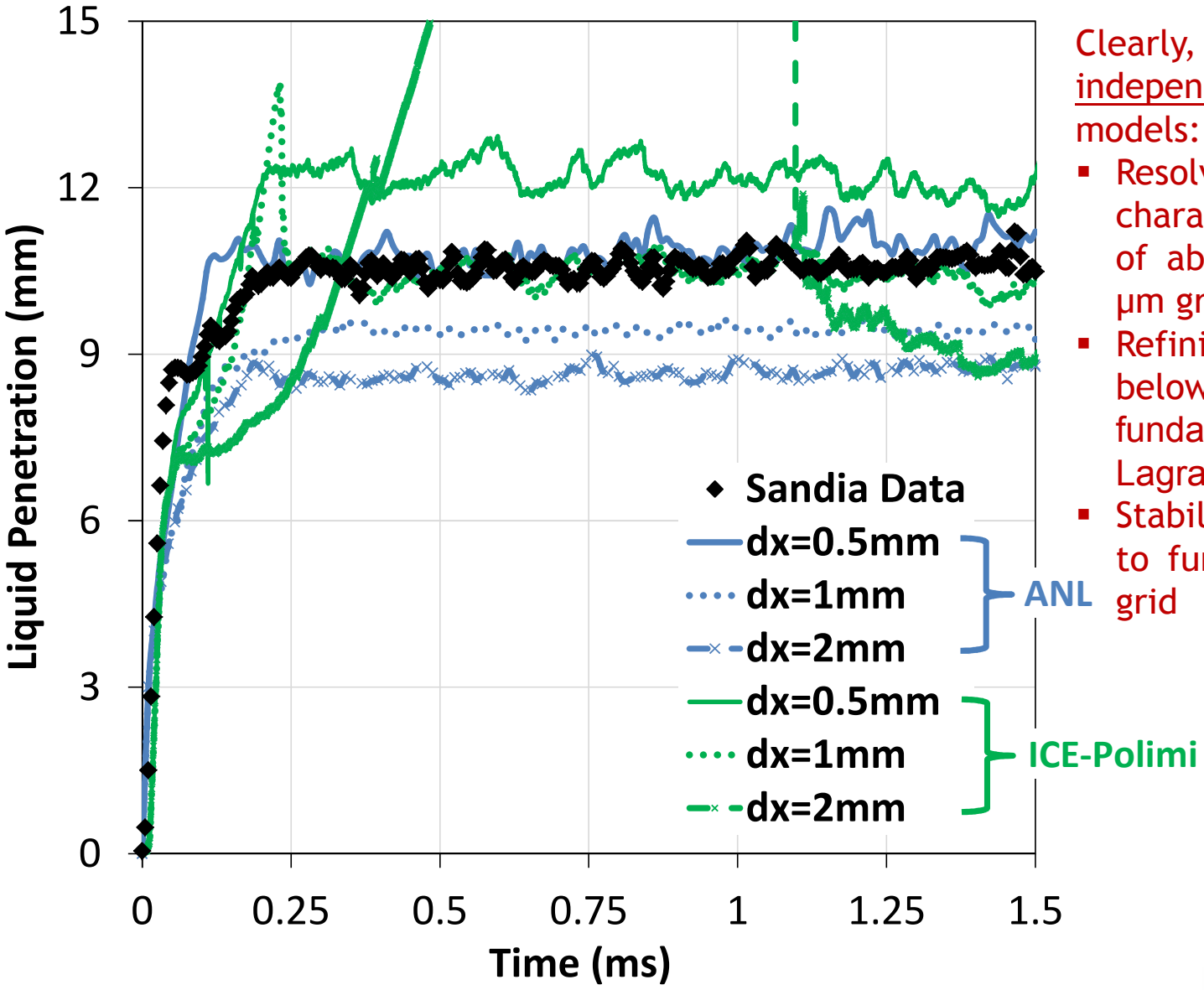


X = 45 mm



Effect of “Grid” Size

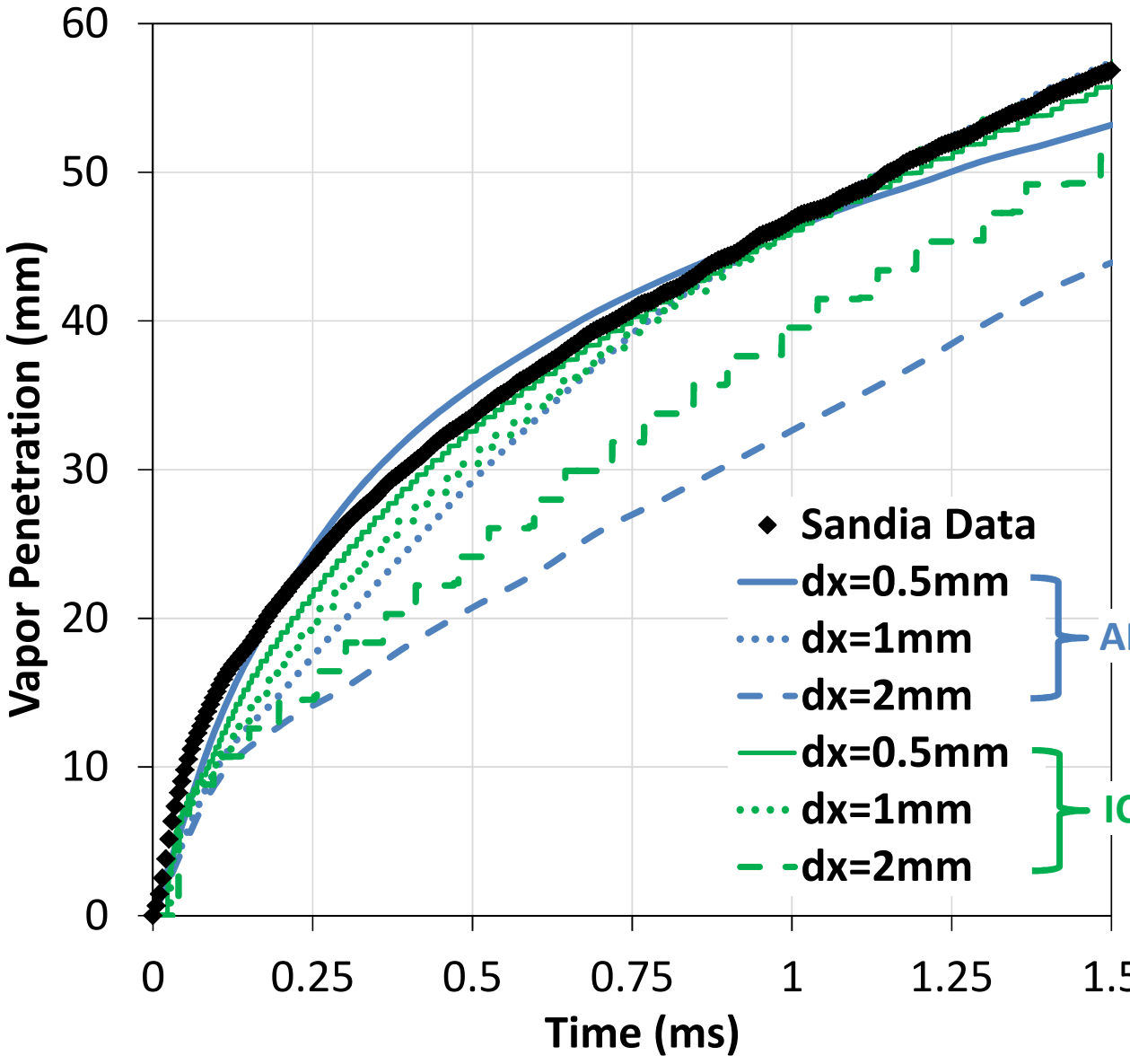
Spray Penetration



Clearly, results are not grid-independent 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

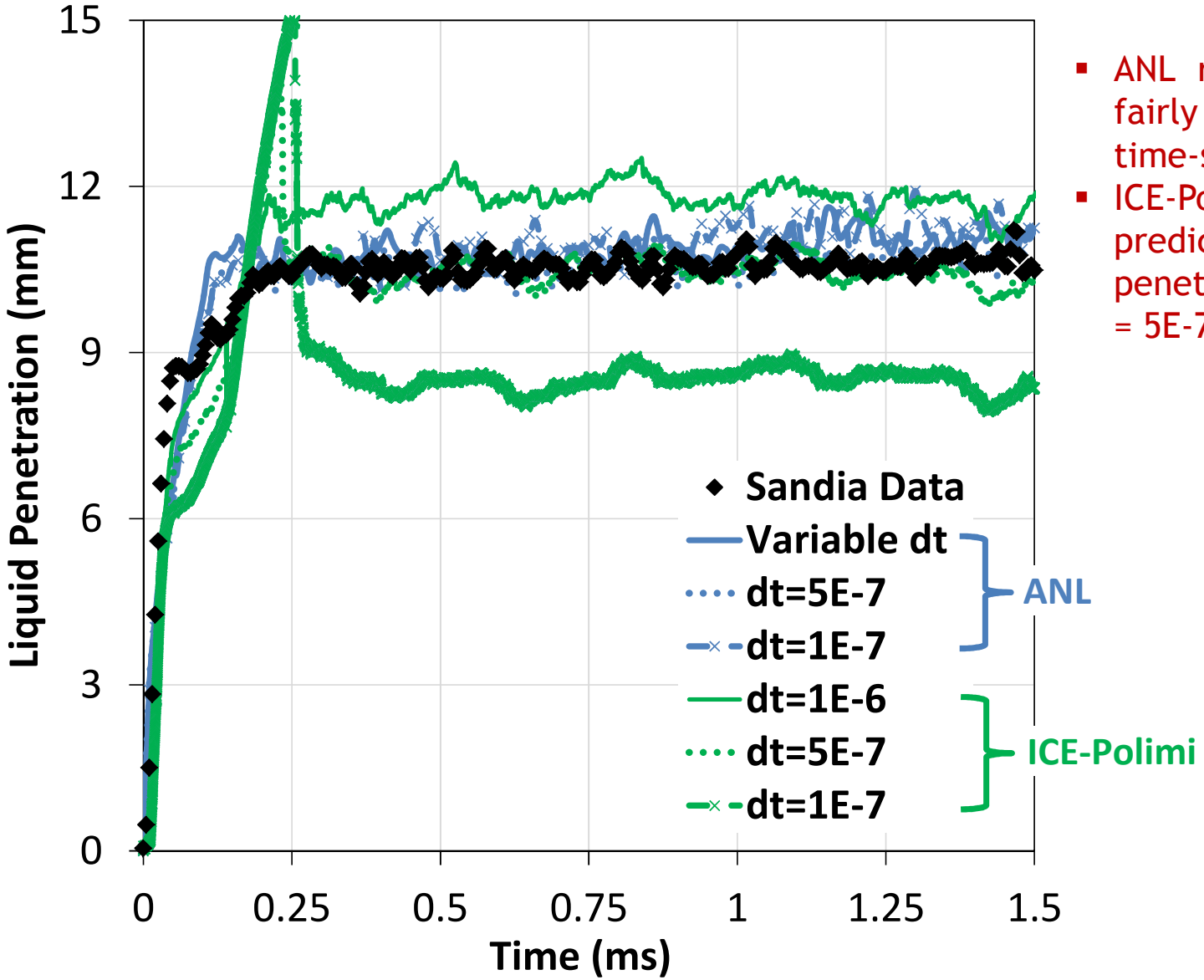


Results are not grid-independent with the RANS models:

- 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?

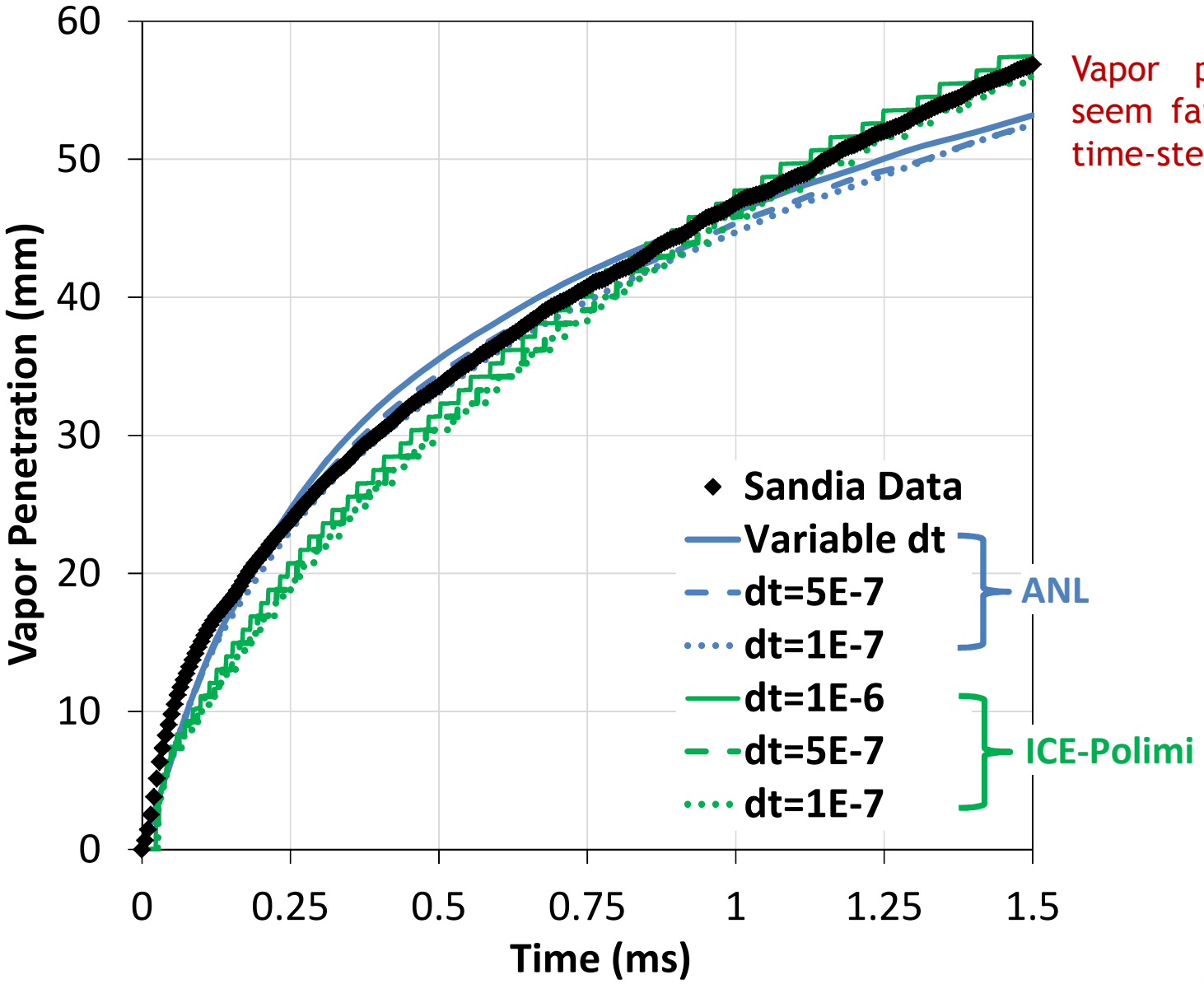
Effect of “time-step” Size

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

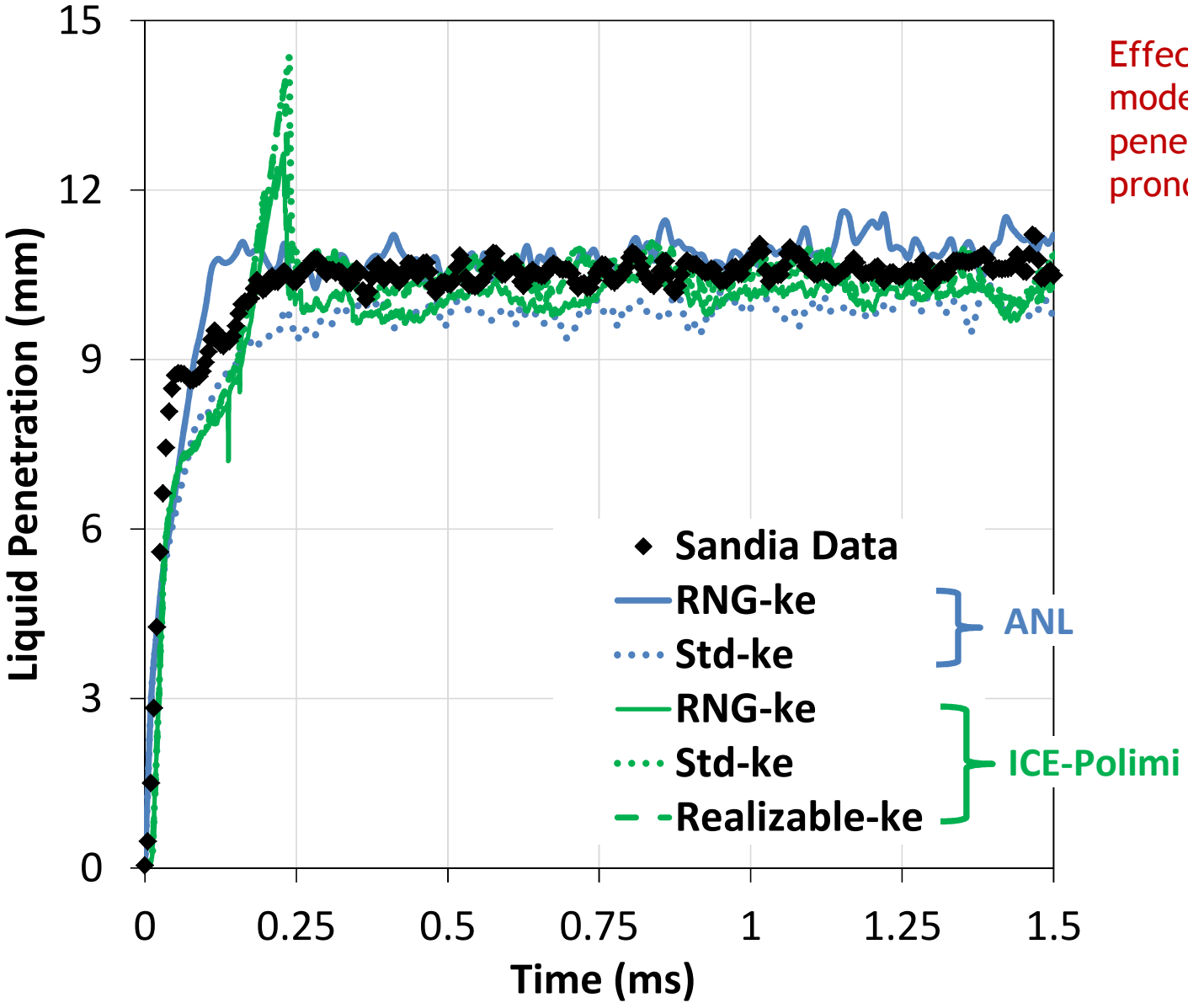
Vapor Penetration



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

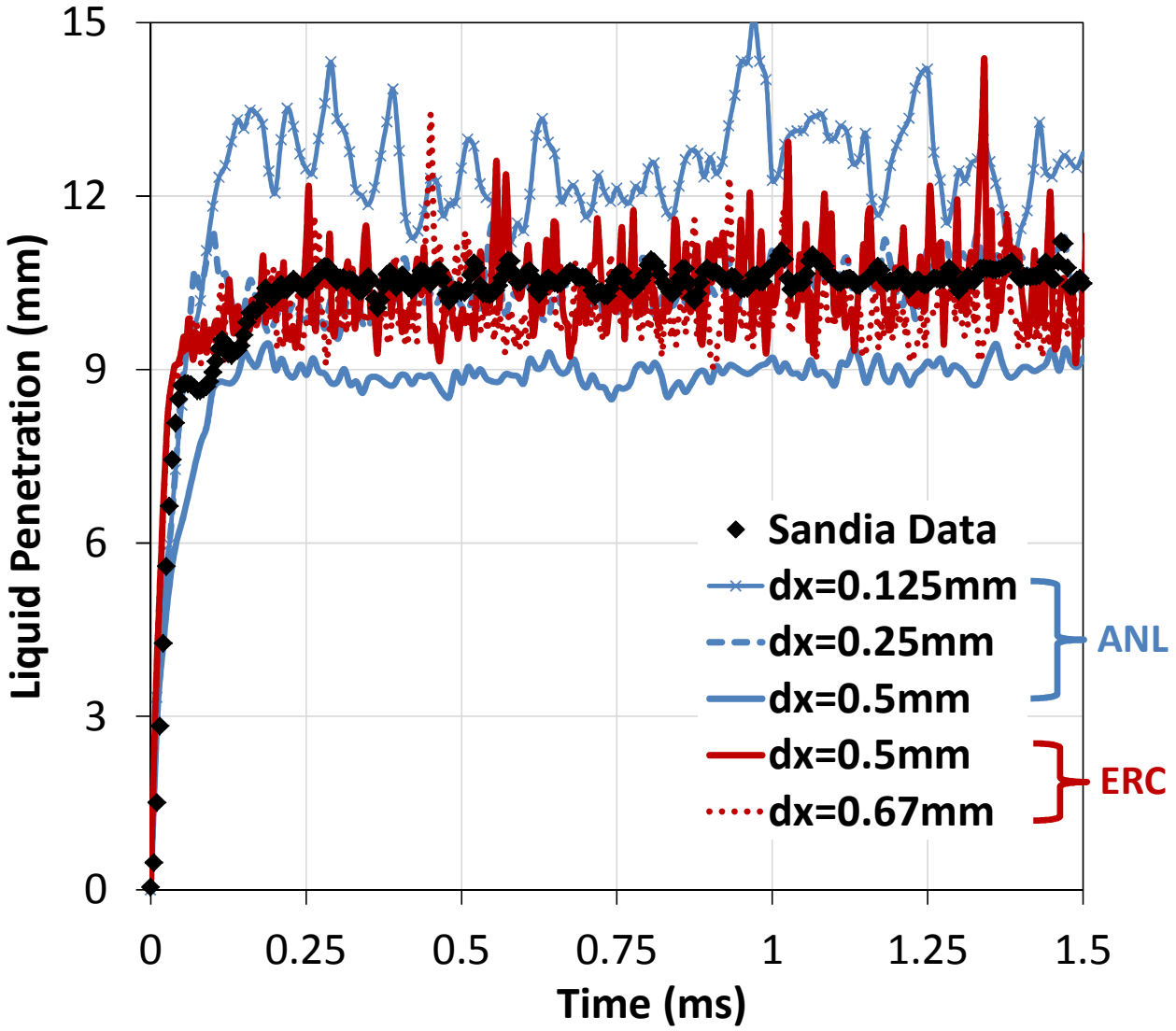
Effect of “Turbulence” Models

Spray Penetration: Different RANS models



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

Spray Penetration: Different LES models

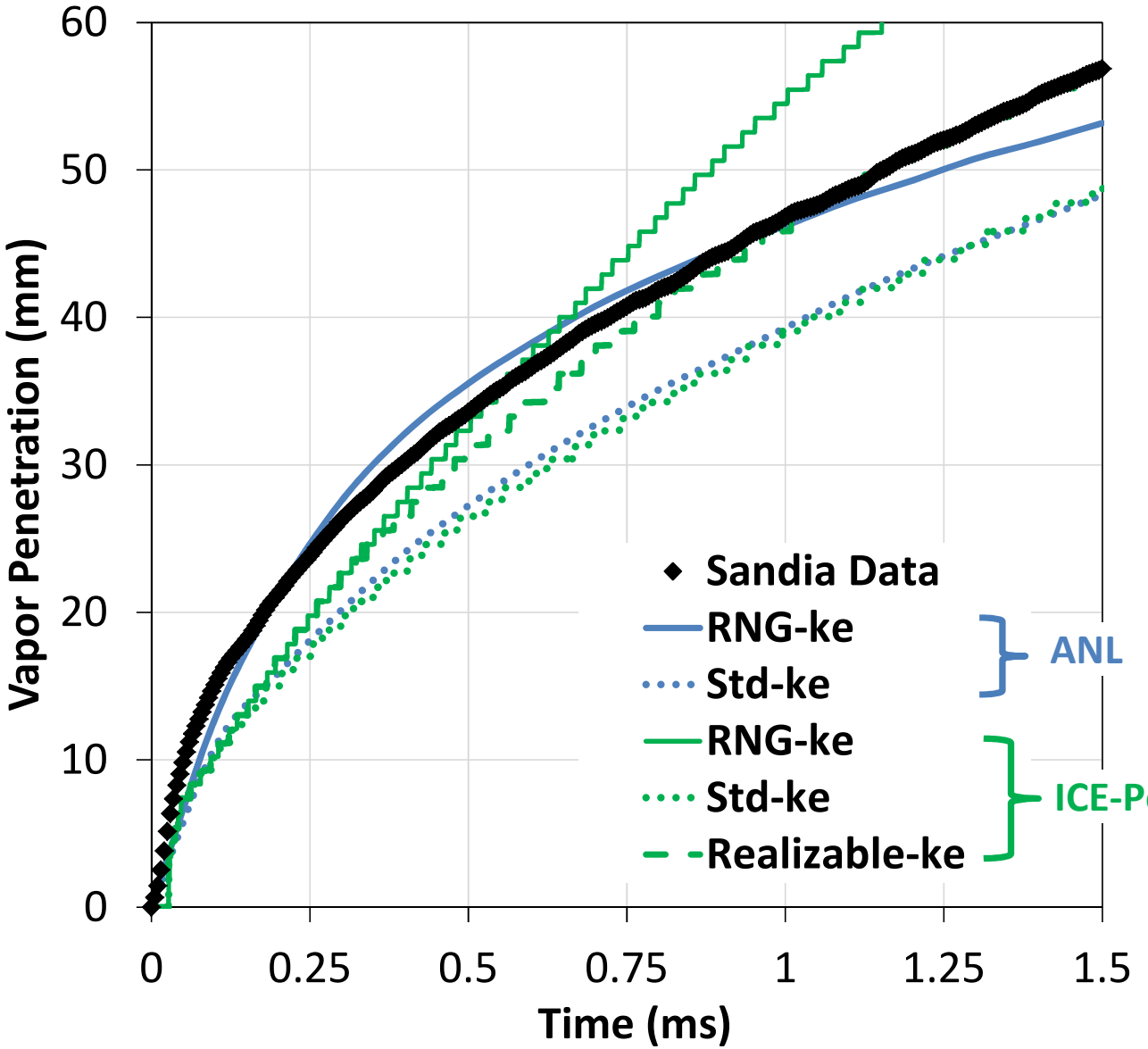


Grid independence on spray penetration observed with ERC-LES model

ANL model:

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

Vapor Penetration



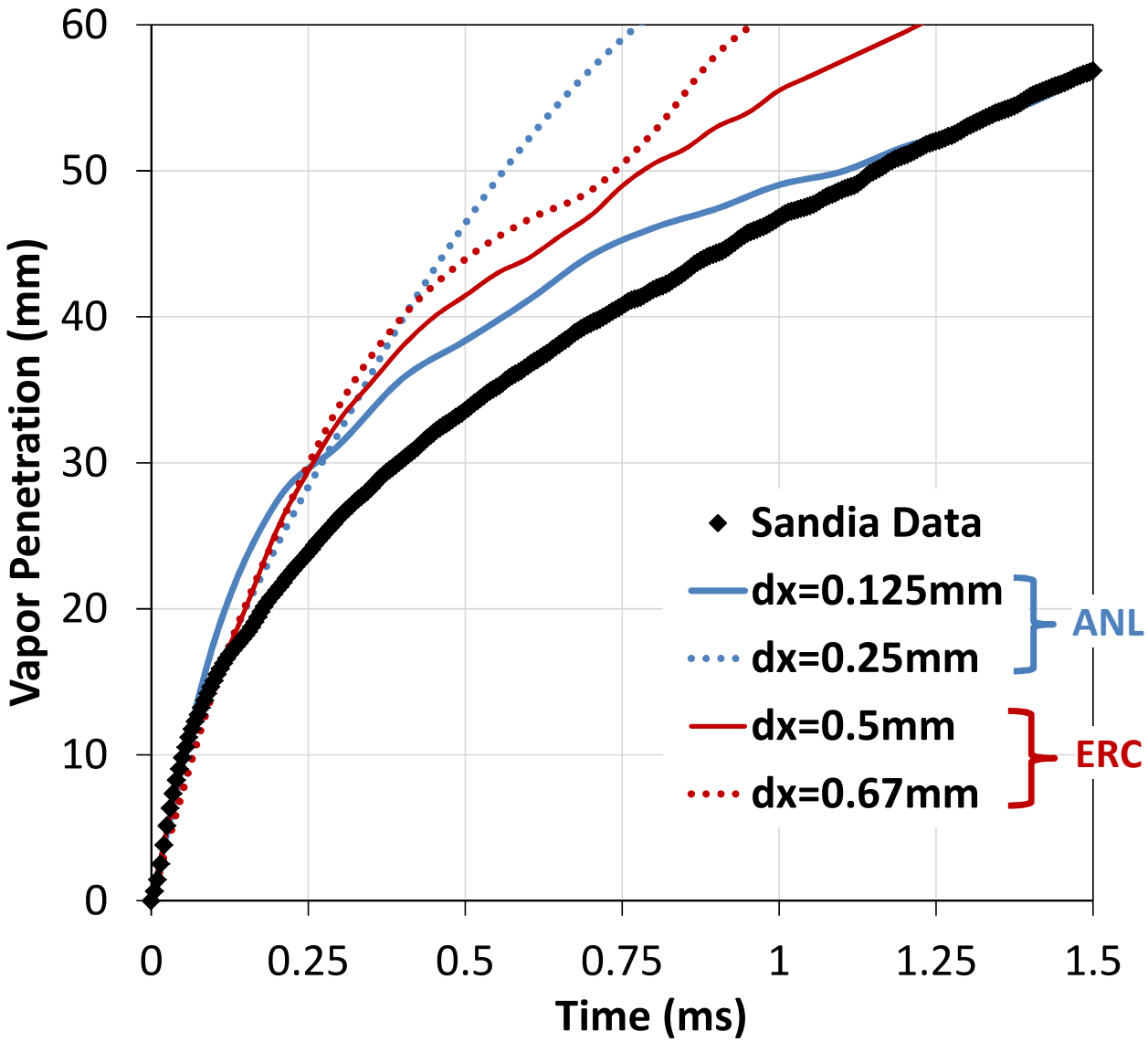
Effect of RANS turbulence models on vapor penetration is much more pronounced

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

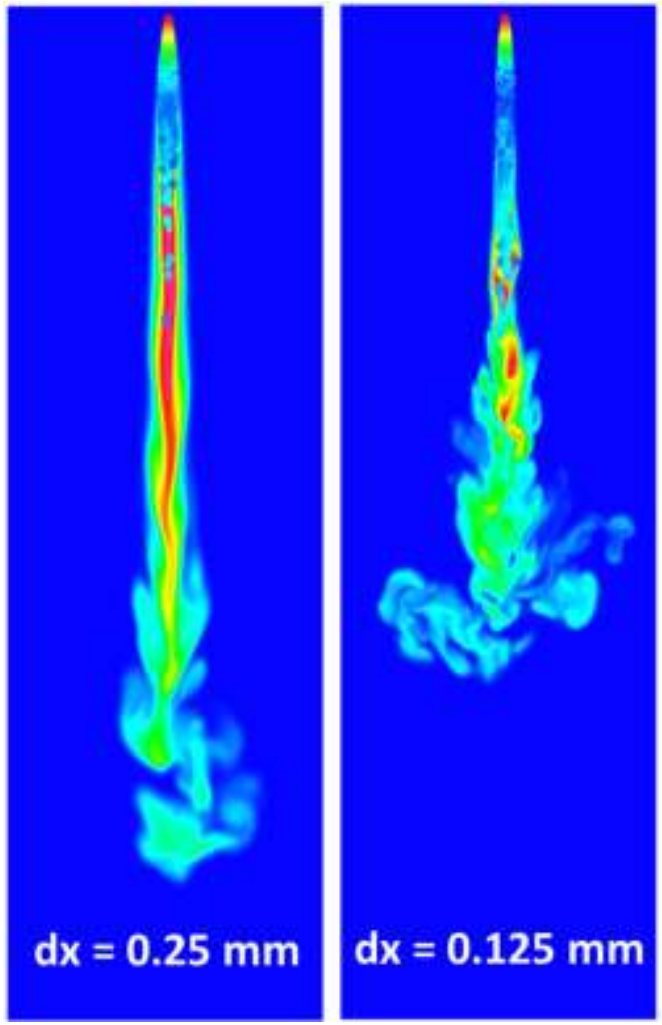


Results are not grid-independent with the LES models also:

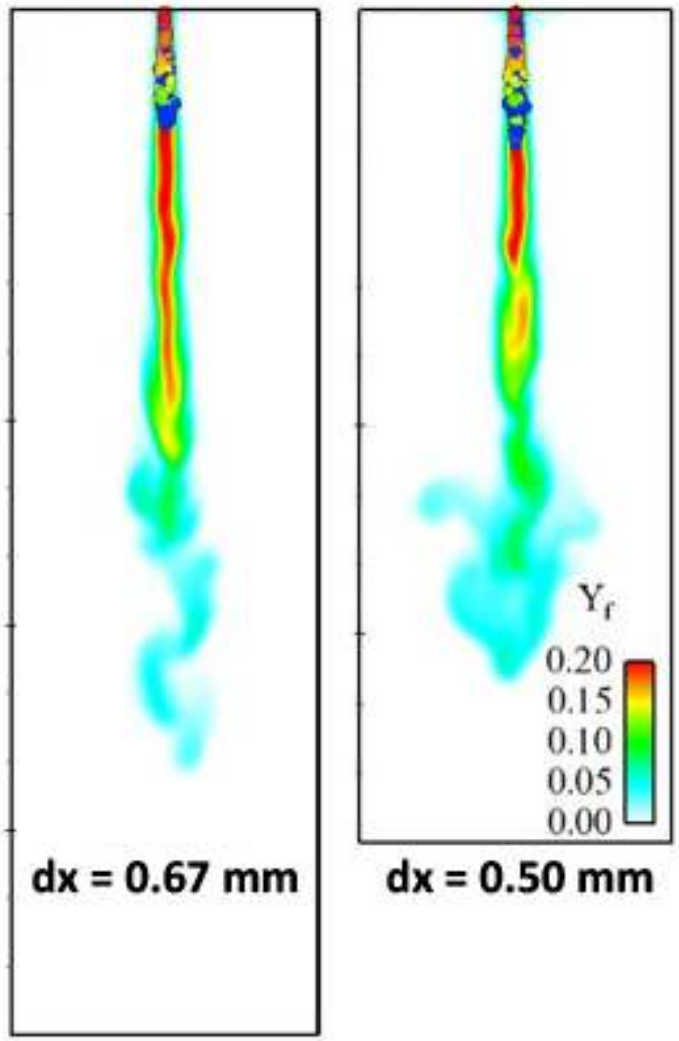
- Vapor penetration decreases with decrease in grid size. This trend is opposite to that observed for RANS simulations
- LES models need to be improved to better predict vapor penetration

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

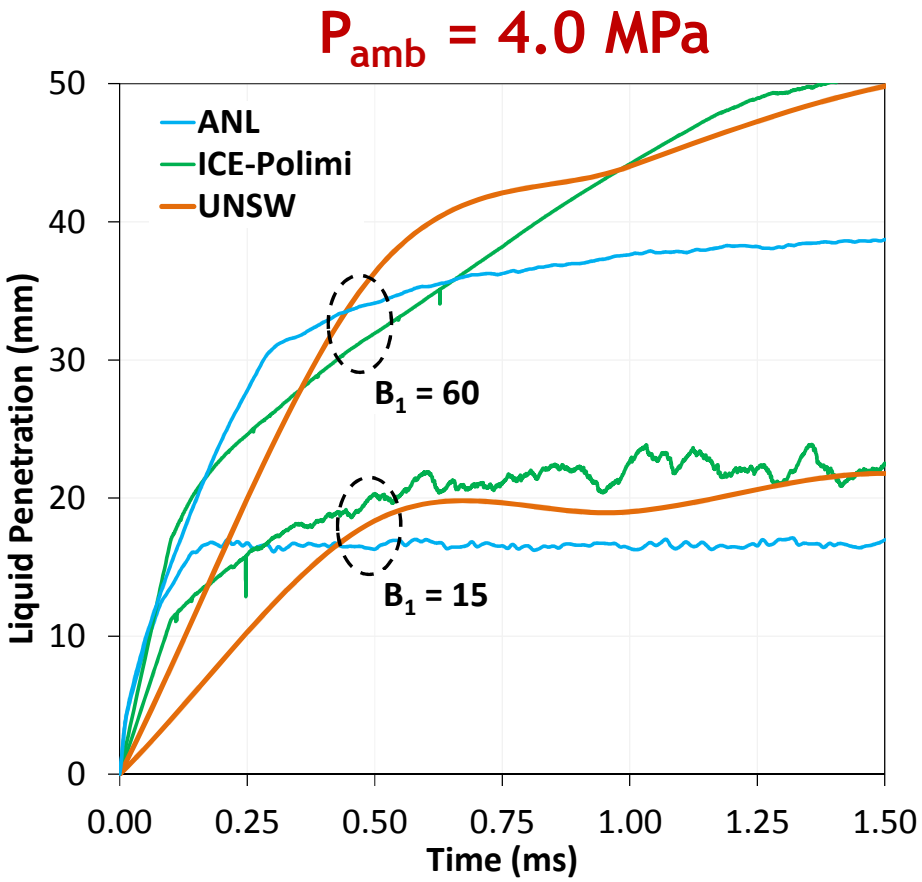
	Case 1	Case 2
Ambient gas pressure	4.0 MPa	8.0 MPa
Ambient gas density	14.8 Kg/m^3 (approx.)	30.0 Kg/m^3 (approx.)

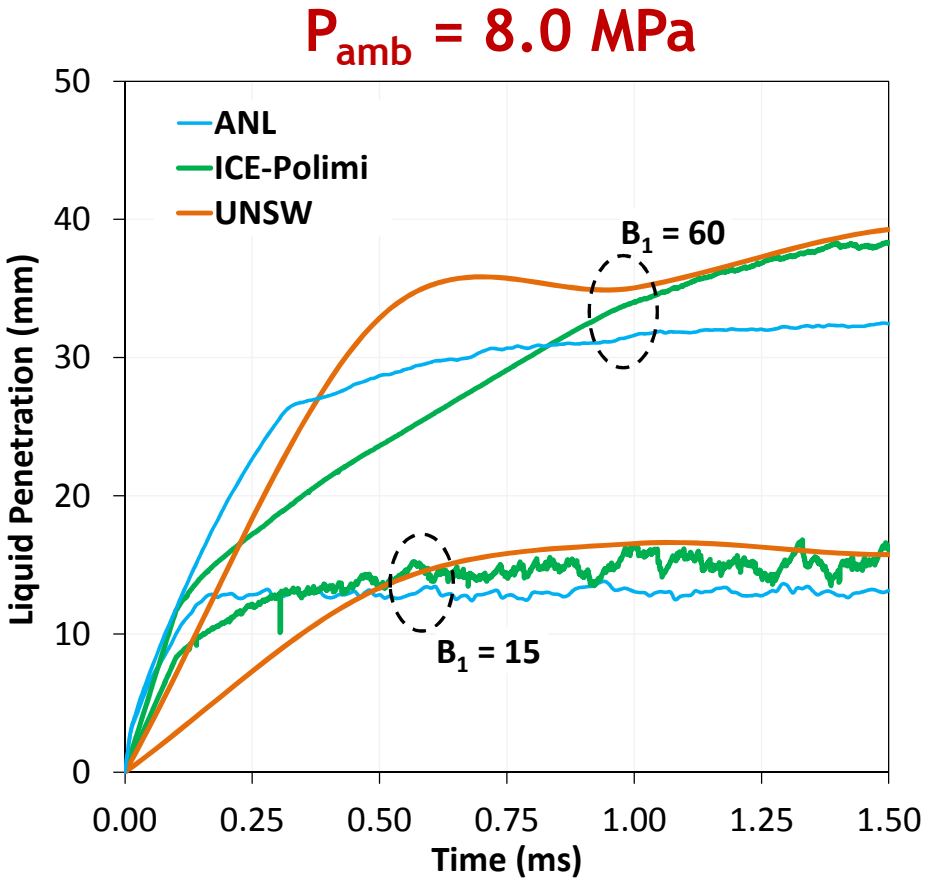
- ❑ Standard k-ε model
- ❑ Blob injection model
- ❑ No collision model
- ❑ Standard drag model
- ❑ PISO time discretization
- ❑ Frossling evaporation model

- ❑ 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

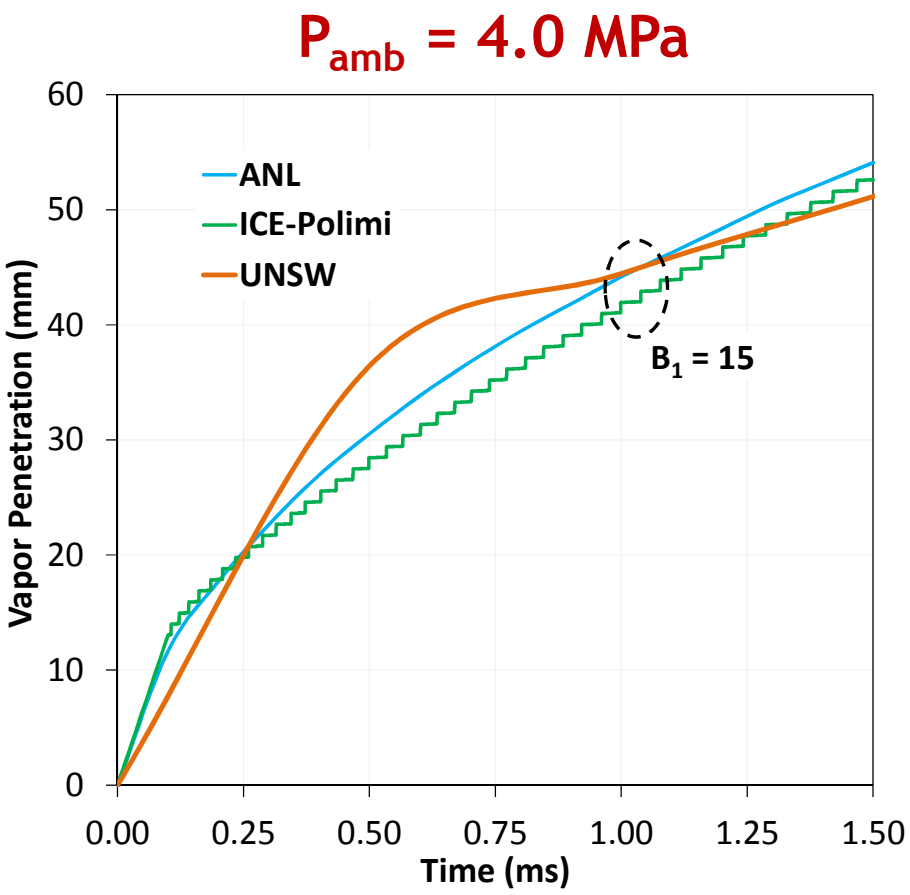
Spray Penetration

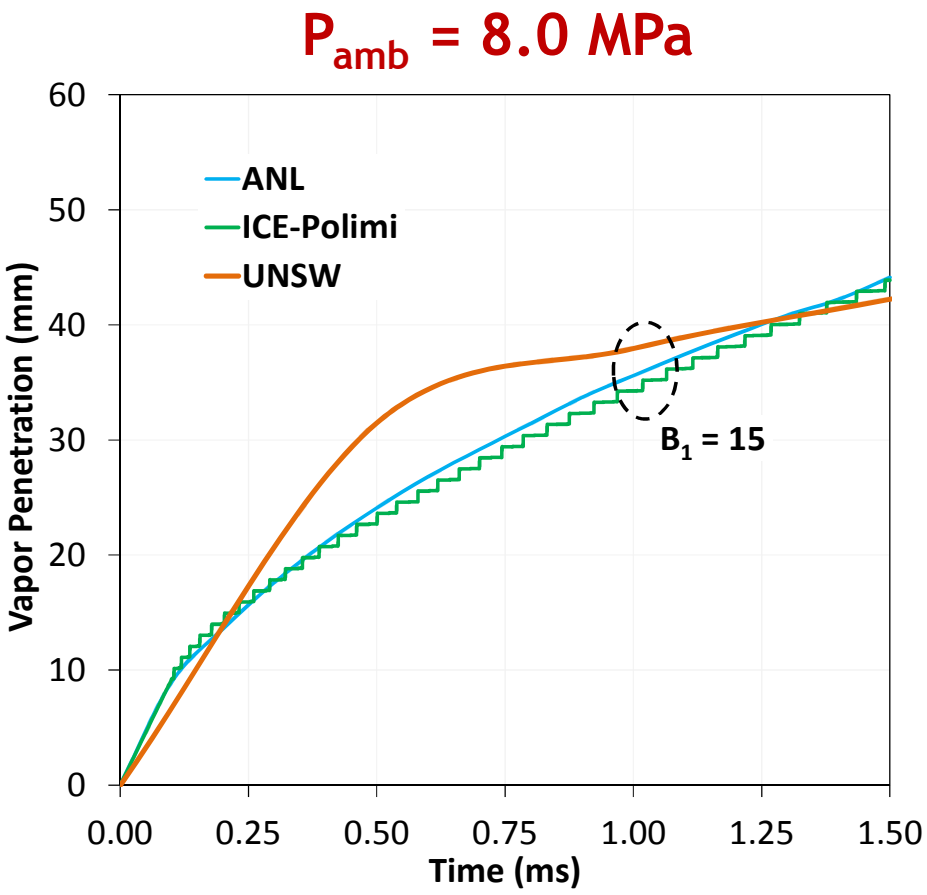




- B1 is perhaps the most influential spray model constant
- Differences in simulation results are very apparent
  - Initial transience is markedly different
  - Different steady state liquid lengths predicted
  - Differences are more pronounced at lower ambient pressure values

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

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