LARGE-EDDY SIMULATION FOR ENERGY CONVERSION IN ELECTRIC AND Argonne COMBUSTION ENGINES (LES4ECE)

COUPLING LAGRANGIAN-EULERIAN SPARK-IGNITION (LESI) MODEL WITH LES COMBUSTION MODELS FOR ENGINE SIMULATIONS

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Abstract:

In this presentation, the coupling of a high-fidelity ignition model (LESI) with combustion models is discussed in detail. The model is part of ongoing ignition research at Argonne National Laboratory, which contributes to several projects and consortiums relevant to internal combustion engine research. LESI relies on a hybrid Eulerian-Lagrangian approach to track the arc and deposit the energy in the corresponding computational cells. First the details of the LESI model, especially its arc tracking capabilities, are discussed. Then, the coupling of LESI to conventional flame propagation models (G-equation, thickened flame model, and well-stirred reactor) is explained in detail. The LESI model is then tested in a combustion vessel and the results show successful spark channel elongation prediction and coupling with the combustion models. Finally, LESI is used to simulate a stoichiometric condition in a DISI engine, where it successfully tracks the arc channel while coupled to the combustion models.

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MOTIVATION AND STATE OF THE ART

https://www.eia.gov/outlooks/aeo/

Gasoline LDVs still Relevant

- Light Duty vehicles are the largest mode of transportation in the US
- Gasoline engines projected to remain relevant by 2050
- Ignition modeling is highly relevant for ignition system design in unconventional modes \rightarrow to reduce CCV

Spark-Ignition (SI) Models and Challenges

- Most popular approaches in industry today rely on a simplistic ignition models.
 - Spherical energy deposition, moves with the flow
 - G-EQ, ECFM, TFM are the most used SI combustion models. WSR used at some conditions.
- Several ignition models available, mainly divided between Lagrangian and Eulerian
 - DPIK, AKTIM, SparkCIMM, ISSIM, etc...
- Several features (circuit modeling, blow-outs/restrikes, radiative & heat transfer losses, plasma properties, etc.)

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2010

- Can negatively impact the ignition model predictivity if missing
- Scarce model validation at challenging operation of interest to industry:
 - High-load SI \rightarrow Impact of turbulence on spark-channel elongation and cyclic variability.
 - Lean/dilute SI \rightarrow Impact of kernel size on lean and EGR dilution limits.
 - Cold-start SI \rightarrow Impact of preferential vaporization and low-turbulence on kernel growth.



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IGNITION MODELING AT ANL – SCOPE OF PRESENTATION

Ignition Modeling at ANL

- 1. Sub-model for early flame growth
 - a. Flame curvature/strain, wall heat loss, etc..
 - b. Integration into established combustion models
- 2. Advanced energy deposition model (LESI)
 - a. <u>Model usability → coupling with established</u> <u>combustion models</u>
 - b. Model development → addition of onboard secondary circuit, short-circuit, and blowout/restrike sub-models



Scope of Presentation

LESI model integration with combustion models

- a. Description of the internal works of the LESI model
 - i. Arc tracking and energy deposition
 - ii. Coupling with combustion models
- b. Combustion vessel results
 - i. Spark channel elongation
 - ii. Flame propagation
- c. LES DISI engine results
 - i. Well-stirred reactor (WSR)
 - ii. Thickened flame model (TFM)
 - iii. G-equation (G-eq) model
- d. Conclusion and future direction





PART I: LAGRANGIAN-EULERIAN SPARK IGNITION (SI) MODEL





LESI MODEL – DEVELOPMENT AND FUNCTIONALITY

History of Ignition Modeling at ANL

- Detailed energy deposition in quiescent conditions
- With correct input (including CHT), can predict ignition success and misfire
- Previous work:
 - Zhang, A., Scarcelli, R., Lee, S., Wallner, T., et al., 2016, "Numerical Investigation of Spark Ignition Events in Lean and Dilute Methane/Air Mixtures Using a Detailed Energy Deposition Model," SAE Paper No. 2016-01-0609.
- LaGrangian-Eulerian hybrid formulation for non-quiescent conditions (LESI)
- LESI is a line-source spark-ignition model developed at Argonne within the Converge framework using user defined functions (UDFs) for the glow phase of ignition
- Previous work:
 - R. Scarcelli, et al. Development of a Hybrid Lagrangian-Eulerian Model to Describe Spark-Ignition Processes at Engine-Like Turbulent Flow Conditions, Journal of Engineering for Gas Turbines and Power 141 (2019), DOI: 10.1115/1.4043397

LESI Features

- Main features:
 - Source energy distributed among the points based on segment length relative to total arc length



LESI MODEL – DEVELOPMENT AND FUNCTIONALITY

LESI Features (continued)

- Main features:
 - Source points move with the flow with limitations
 - Elongation limited to model the spark channel impedance to flow
 - Source point velocity affected by local and adjacent point velocities
 - End points cannot detach from the electrode surface
 - Line gets truncated if non-end point gets too close to the electrode surface

End point moved to the closet point and all the points between the previous end point and the current end point are deleted





End points move along the electrode boundary surface but never detach



LESI MODEL – DEVELOPMENT AND FUNCTIONALITY

LESI vs Typical Energy Deposition Modeling

Schlieren images from Dr. Lee (MTU)

- Significant improvement in arc tracking by introducing LESI model UDFs
 - Improvement in energy deposition distribution, directly due to the improvement in arc tracking
 - Potential to help evaluate operating conditions that pose challenges on ignition success



- Advantages of LESI over older models:
 - No need to predefine ignition criteria
 - No need to predefine transition from kernel to flame
 - Accounts for breakdown perturbation



LESI MODEL – COUPLING WITH COMBUSTION MODELS

Arrhenius Based Models (WSR and TFM)

- Coupling seamless through temperature rise from energy deposition
 - Ignition model generates a T rise through an energy source equivalent to ignition energy generated by experiment, regardless of ignition shape
 - Rise in Arrhenius term which lead to reactant consumption
- Flame sustains itself through species and heat diffusion
- TFM delayed to ensure flame propagation and avoid premature quenching (~2 CA for engines)

 $\frac{\partial}{\partial t} \left(\rho \left(e + \frac{1}{2} u_k^2 \right) \right) + \frac{\partial}{\partial x_i} \left(\rho u_i \left(e + \frac{1}{2} u_k^2 \right) \right) =$ $-\frac{\partial}{\partial x_{i}}(u_{j}P) + \frac{\partial}{\partial x_{i}}(u_{i}\sigma_{ij}) + \frac{\partial}{\partial x_{i}}\left(K\frac{\partial T}{\partial x_{i}}\right) + \frac{\partial}{\partial x_{i}}\left(\rho D\sum_{m}h_{m}\frac{\partial Y_{m}}{\partial x_{i}}\right) + S.$

Insert a volumetric source term (J/m³s) in specified computational cells

G-Eq Model

- Temperature cut-off approach where g=0 iso-surface is initialized when T>3000 K
 - Value of cutoff temperature can be tuned to improve initialization
 - Weak influence
 - Immediate turbulent flame propagation is assumed per S_t
 - Turbulence/flame kernel interaction
 - Could benefit from accounting for laminar flame formation and growth
 - Leads to faster flame propagation





PART II: COMBUSTION VESSEL





COMBUSTION VESSEL - SETUP

Experiment – MTU Ignition Vessel

- Constant volume ignition vessel at Advanced Power Systems (APS) Laboratory at Michigan Technological University (MTU)
- 1.1 L vessel, allows mounting spark plugs, injectors, and others
- Provides optical access to record PIV and Schlieren images
- Can handle temperatures up to 2100 K and pressures up to 345 bar
- Contains a shrouded fan that directs the flow towards the spark plug
- 8 blades with 25.4 mm outer diameter
- Controlled by a 12V motor with a control system that maintains fan speed at set value

Simulation

- Converge 3.0.16 with GRI-MECH 3.0
- Grid ranges between 1 and 0.0625 mm
 - Consistent with typical engine grid sizes
- RANS k-e RNG and LES dynamic structure model
- Propane with Eq. Ratio=0.9 and 20% EGR by mass
- Fan speed = 6000 rpm

Property	T (K)	P (bar)	Glow Energy (mJ)	Gap Vel. (m/s)
Value	423	16	30	2



COMBUSTION VESSEL – QUALITATIVE COMPARISON



WSR and TFM

- Successful coupling of LESI with TFM and WSR
- LESI compatible with different turbulence models and grid sizes
- Results validated versus experiment
- TFM turned on when ignition ends
 - Improved flame propagation vs WSR





Successful coupling of LESI with G-eq

- S_t in RANS: Peters with g' and in LES: Pitsch
 - Default values for b1 and b3

G-eq

 Flame propagation overestimated versus experiment in both longitudinal and lateral directions

Schlieren images from Dr. Lee (MTU)

 Spark channel elongation comparable between G-eq and WSR
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PART III: DIRECT-INJECTION SPARK-IGNITION (DISI) ENGINE





DISI ENGINE – SIMULATION AND EXPERIMENT SETUPS

Experiment – Sandia DISI Engine

- DISI 4-stroke engine at Sandia National Laboratory
- 4 valve engine, with variable intake flow configuration (swirl and tumble)
- Datasets include PIV/schlieren/direct flame imaging

Simulation

- Converge 3.0.16 with E30 defined as composite
- Grid ranges between 4 and 0.125 mm
- AMR turned on for SGS V and T at 0.5 mm
- LES dynamic structure model
- Tabulated laminar flame speeds

Property	Value	
Bore	86 mm	
Stroke	95 mm	
Connecting rod	166.7 mm	
Crank speed	1000 rpm	
Compression ratio	12	
Intake P	~46 kPa	
SOI/num of injections	-298º aTDC/3	
Global Eq. Ratio	1.0	
Injection duration/mass	2.622 CAD/5.93 mg	
Time between injections	15 CAD	
ST	-12.6º aTDC	
Ignition energy	~106 mJ	
BD source	Stationary cylinder (20 mJ)	





Implemented in engine and boundary list updated





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DISI ENGINE – RESULTS – WSR – BASELINE CASE

WSR

- Preliminary results with RANS show less CCV compared to LES (as expected)
- Reaction multiplier varied to tune pressure traces
- Coupling with WSR successful
- Model tuned for peak pressure

5.0e+02

Time: -19.99 (CAD)

- Heat release overestimated at later times
- LESI arc tracking and kernel formation behaving as expected

TEMPERATURE

15002000

3.0e+03





LESI Model

- Endpoints always attached to the electrodes
- In this cycle, arc pushed into the spark plug gap, rather than away
 - Depends on the local velocity field



DISI ENGINE – RESULTS – TFM

β tuning is not necessary if TFM relies on a dynamic formulation

10

-10

10

ime: -19.97 (CAD

Apparent Heat Release Rate (TFM with LESI)

Crank Angles (Degrees)

Wrinkling Factor E

0e+00 6 8 10 1.5e+01

EXP AVG

LES AVG

TFM

- Reaction rate sensor model with Jaravel's correction
- 10 cells across the flame front (~10% of flame thickness)
- Charlette's efficiency function model with β =0.62
- Turned on at -10° aTDC
- TFM improves pressure trace and heat release rate, compared to only WSR
 - Thickening factor within reasonable range for engines
 - Wrinkling factor significant for flame propagation







Thickening factor F applied in relevance to the sensor



DISI ENGINE – RESULTS – G-EQ

G-Ea

17

- Pitsch expression for turbulent flame speed, tuned b1 and b3
- CEQ in burnt and flame regions (simplified mechanism)
 - Burnt region showing different temperature behavior compared to WSR/TFM
- Global metrics show that G-Eq at this operating point is not very sensitive to the fidelity level of the ignition model
 - Fast and convenient approach for OEMs



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02 (bar)

) Lessare 10

-10

Time: -19.97 (CAD)





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DISI ENGINE – RESULTS – FLAME INITIALIZATION

Plasma and Arc Tracking

- Engine operating condition characterized by swirl and very low (almost no) tumble
 - Spark channel does not follow a dominant displacement/elongation direction (unlike with tumble)
- <u>LESI successfully models the</u> plasma/arc shape, location, and elongation
- Traditional spherical models do not track the arc
 - Leverage LESI's accurate arc tracking in high turbulence/high CCV conditions (next step for LESI)

Kernel Formation

 Kernel formation in G-eq model faster than in WSR and TFM (as expected)

Experimental images from Dr. Sjöberg (Sandia National Lab)



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PART IV: CONCLUSION





MAIN CONCLUSIONS, FINDINGS, AND CONTRIBUTIONS

Conclusions

- LESI is a high fidelity spark ignition model which relies on Lagrangian arc tracking and Eulerian energy deposition in the equivalent computation cells
 - Several features: distributed energy source, end point attachment, end point truncation, center point elongation
- Successful coupling of a hybrid Lagrangian-Eulerian high fidelity spark ignition (LESI) model to typical flame propagation models (TFM, G-eq)
 - Initial testing in combustion vessel \rightarrow validation of flame propagation and spark channel elongation
 - Main testing in DISI engine:
 - Validation of results against experiment in global and spatial metrics, such as pressure, heat release, and temperature contours
 - Spark channel elongation successfully modeled
 - LESI model arc tracking sensitive to velocity field fluctuations → impactful in high turbulence/high variability conditions (such as high load and lead/dilute, which are of interest for OEMS)
- LESI is an advanced energy deposition model, which is now available for engine simulations and usable with both RANS and LES flame propagation models, as shown in this work



NEXT STEPS AND OTHER WORK

Next Steps

- Assess the impact of the high fidelity LESI model on CCV in engine simulations
 - Requires a different operating conditions \rightarrow very likely high load or lean dilute
 - A high level of turbulence in the engine cylinder would be desirable
 - LESI accounts for the impact of the flow field variability on the ignition event
 - LESI can account for any spatial variability on the ignition event
 - Turbulence, eq. ratio stratification, dilution, etc...

Additional on-going LESI Work

- Work being done through a CRADA with Stellantis (formerly Fiat-Chrysler Automobiles) main goal is to increase the fidelity of the LESI model by:
 - Validation of the model in different cross-flow conditions → to account for the ability of LESI to handle different flow fields (completed)
 - Account for further physical phenomena such as short-circuit and blowout/restrike
 - Incorporate seamless sub-models into the main LESI formulation to truncate the Lagrangian points as needed to model an arc short or restrike
 - Relies on an onboard secondary circuit which feeds electrical data (current, energy, spark channel resistance, etc.) to the short-circuit and blowout/restrike sub-models.



THANK YOU!

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