

Project 029(B) Area 5: Development of Spray Models for the Description of Multicomponent Jet Fuel Effects

Stanford University

Project Lead Investigator

Matthias Ihme
 Assistant Professor
 Department of Mechanical Engineering
 Stanford University
 488 Escondido Mall, Building 500, Room 500A, Stanford, CA 94304
 650-724-3730
mihme@stanford.edu

University Participants

Stanford University

- P.I.(s): Matthias Ihme, Assistant Professor
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Investigation Team

- Matthias Ihme, Assistant Professor
- Tasks: principal investigator, oversees project progress, coordination with research teams from other FAA-NJFCP subject areas, presentation of research findings
- Pavan Govindaraju: Graduate student
- Development of multicomponent evaporation model
- Peter C. Ma: Graduate student
- Perform detailed simulations and validation studies of level-set/volume-of-fluid method to predict primary and secondary breakup characteristic; validation against experiments performed at Purdue University.
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Project Overview, Approach, and Accomplishments

The objective of this effort is the development of computational models for the reliable prediction of the primary breakup and droplet evaporation of multicomponent reference fuels. Currently, the prediction of primary breakup relies exclusively on phenomenological models that have been derived from linear stability arguments. While these models provide a rudimentary representation of liquid inertia, surface tension, and aerodynamic and viscous forces, these models are not predictive and rely on empirical input parameters. In addition, the gas-fuel deposition and the evaporation rate of the liquid fuel critically affect the ignition, the flame-stabilization, and the pollutant formation. However, the evaporation process requires the consideration of intra-droplet processes, the gas-phase transport at the droplet boundary, and the description of the droplet interface for subcritical conditions. Since the reference fuels consist of different components, covering a wide range of vaporization conditions, a multicomponent evaporation formulation is required.

The overall objectives of the proposed research are:

- (i) Develop surrogate representations for multicomponent fuel-evaporation of the three reference fuels



- (ii) Develop and implement multicomponent evaporation model into Lagrangian particle model
- (iii) Perform parameter simulation to assess effects of spray-evaporation on combustion, flame stabilization, and flame structure
- (iv) Perform LES simulation of RTS and RGTC. Compare modeling results against experiments and evaluate capability of currently employed phenomenological RT/KH breakup models.

Task: Modeling of multicomponent droplet evaporation

Introduction

Computational approaches to multicomponent droplet evaporation introduce challenges in generalizing to arbitrary fuel blends due to the vast number of assumptions that are being introduced to describe evaporation and composition. Some models [3] simplify on the computational cost by using a distribution-weighted average of component properties without a physical justification for the choice of the distribution. Other methods [2,3,6,11] arbitrarily generalize existing physical property correlations to fractional carbon numbers. In addition to this, current literature is restricted to specific families of components which is an infeasible approach for aviation fuel blends which not only have a high species count but also contain components belonging to widely different families of organic compounds. This motivates a generalized approach where the lack of experimental data is taken to be inevitable and physical properties must be calculated from first principles.

Measurements from distillation and chromatography provide information regarding the molecular weight and functional groups present in compounds, constituting a particular fuel blend. The results presented utilize the fuel descriptions provided in [12]. Also, [1] and [4] describe methods to estimate physical properties of a compound based on the functional groups present in it. To evaluate how suitable the above methods are in calculating multicomponent fuel evaporation characteristics, we need to utilize a highly accurate evaporation model. UNIFAC [5] is a method used to calculate interaction coefficients and is also based solely on the functional groups present in each component. Note that the method described in [1] is compatible with the UNIFAC model and thus enabled the two to be coupled in the simulation code used for obtaining results. Preliminary evaporation studies have been performed on Jet-A and JP-8.

Basic Equations and Approximations

A computational study was performed using the UNIFAC non-ideal evaporation model. Despite the usage of an interpreted language (MATLAB), runtime is of the order of a second for droplet evaporation in fixed ambient conditions, making it a feasible candidate for other codes like reactive flow solvers which utilize an evaporation module. The focus in the following section will however be only on evaluating the effectiveness of this group contribution method in predicting droplet evaporation characteristics of fuel blends.

The evaporation rate is calculated on a per-component basis. A one-dimensional version of this equation is presented in [6] and is commonly referred to as DCM (Discrete Component Model). The current approach is also the multicomponent model implemented in ANSYS Fluent.

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$$\frac{dm_i}{dt} = -4\pi r^2 (MW_i) k_c (C_{i,s} - C_{i,\infty}) \quad (1)$$

where r is radius of the droplet, MW is the molecular weight of species and k_c is the mass transfer coefficient, which in turn is given by

$$k_c = (Sh)(D_i)/2r \quad (2)$$



where Sh is the Sherwood number (can be expressed as a function of Reynolds and Prandtl number), D_i is the diffusion coefficient of species i . Also, for a droplet temperature T_d , the concentration of species at the surface $C_{i,s}$ is evaluated as

$$C_{i,s} = \gamma_i x_i p_{sat,i} / RT_d \quad (3)$$

where p_{sat} is the saturated pressure, γ_i is the activity coefficient, and x_i is the mole fraction of species. Similarly, $C_{i,\infty}$ stands for the far-field equilibrium concentration of the droplet species in the gas phase.

The change in temperature is calculated using the following equation.

$$\frac{dT}{dt} = \sum_i \frac{dm_i}{dt} L_{v,i} + \frac{2\pi(Nu)k_{air}(T_{amb} - T)}{m_d c_{l,m}} \quad (4)$$

where $L_{v,i}$ is the latent heat of evaporation, Nu is the Nusselt number (which can also be expressed as a function of the Reynolds and Prandtl number), k_{air} is the thermal conductivity of the surrounding medium (air in this case), T_{amb} is the ambient temperature, m_d is the mass of the droplet and $c_{l,m}$ is the mole fraction weighted average liquid specific heat capacity of the drop. Time integration was done using 'ode23' since the equations are stiff, especially as temperature of drop approaches the ambient temperature. The Prandtl number was assumed to be a constant, with a value of 0.7 and the following correlations from [7] have been used for calculating the Nusselt and Sherwood numbers:

$$Nu = 2 + \frac{0.555 Re^{0.5} Pr^{1/3}}{1 + 1.232(Re Pr^{4/3})^{0.5}} \quad (5)$$

$$Sh = 2 + 0.6 Re^{0.5} Pr^{1/3} \quad (6)$$

One of the key ideas we present is to use UNIFAC to calculate the activity coefficient. This quantity is a function of the entire mole fraction vector and thus makes this a non-linear problem. In addition to this, we require the physical properties as functions of temperature based only on the knowledge of functional groups and this is achieved using group contribution method [5], which also bases itself on the same functional group definitions as UNIFAC.

There is no known accurate method to estimate binary diffusion coefficients using the primary and secondary functional groups of [1]. For this purpose, the method due to Lee and Wilke [8] is used which yields D_i as a function of the Van der Waals Radius. An intermediate step for calculating the collision integral Ω_D is from [9]

$$\Omega_D = \frac{A}{(T^*)^B} + \frac{C}{\exp(DT^*)} + \frac{E}{\exp(FT^*)} + \frac{G}{\exp(HT^*)} \quad (7)$$

where $T^* = \epsilon/k_B T$.

UNIFAC is based on splitting the activity coefficient calculation into a combinatorial (γ_i^c) and residual component (γ_i^r). Both contributions are totally determined by the three parameters, viz., group surface area parameter R , group volume contribution Q and the binary interaction parameter which is related to the interaction energy.



Results and Discussion

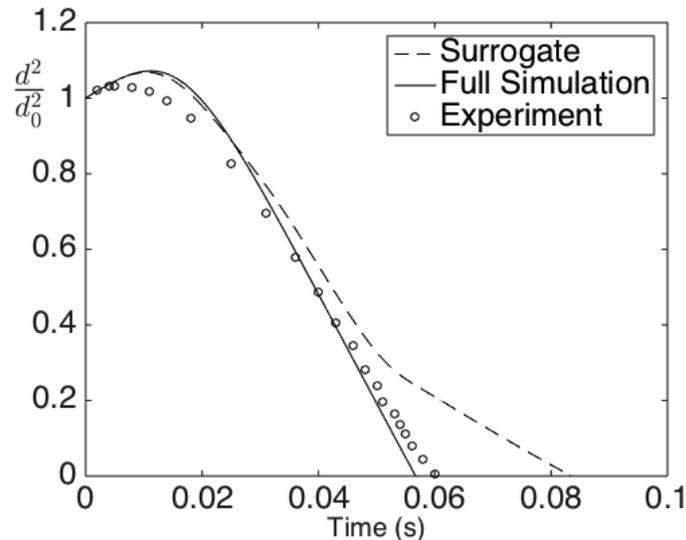


Figure 2: Comparison between quiescent Jet-A experimental evaporation data [2], computational results from group contribution using UNIFAC activity coefficients utilizing the full and surrogate (Jet A POSF 4658 2nd generation) description presented in [12,16]. Initial droplet diameter = 100 μ m, ambient temperature is 800K, initial droplet temperature = 298 K and ambient pressure = 1 bar

Figure 2 shows reasonable agreement between experimental data and the proposed method for evaporation calculations. Further relaxation of assumptions is possible and since Jet-A predominantly consists of non-polar molecules, the same simulation was run with both non-ideal and ideal model, the latter just assumes an activity coefficient of 1 for every component. An error of 0.8% was observed in the evaporation time for the same case. Thus, it is suggested that an ideal evaporation model be used when computational cost is a constraint.

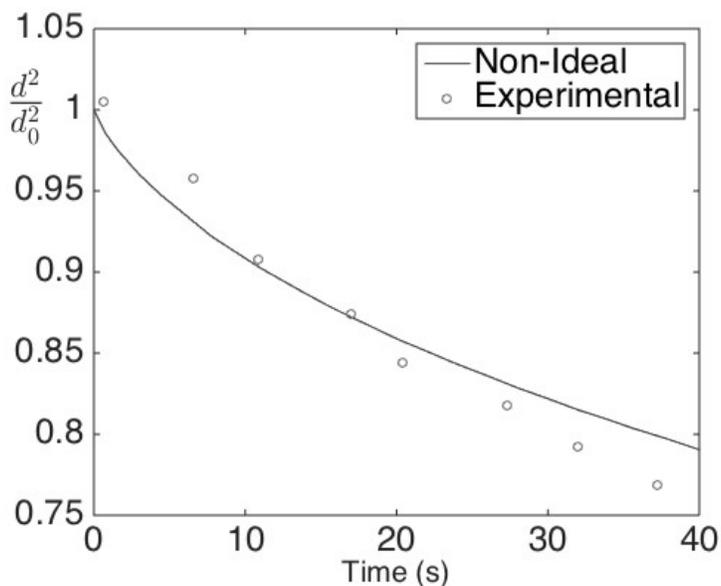


Figure 3: Comparison between JP-8 experimental evaporation[2] and computational results from group contribution using ideal evaporation. Initial droplet diameter = 639 μ m, ambient temperature = 298K, initial droplet temperature = 298 K, ambient pressure = 1 bar, relative velocity =

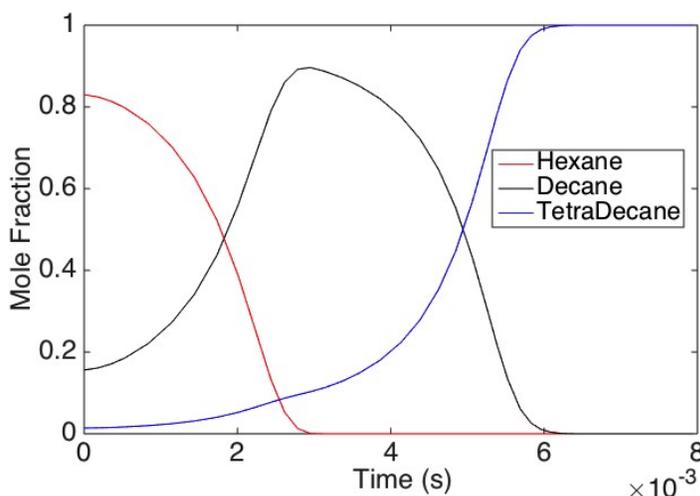


Figure 4: Computational results for 3-component gasoline evaporation surrogate[11] from group contribution using ideal evaporation with 3-quasicomponent model data [11]. Initial droplet diameter = 20 μ m, ambient temperature = 450K, initial droplet temperature = 298 K, ambient pressure = 3 bar, relative velocity = 10m/s

Outreach Efforts

N/A

Awards

N/A

Student Involvement

N/A

Publications

P. Govindaraju, Q. Wang, and M. Ihme, *Multicomponent Droplet Evaporation using Group Contribution Methods with Application to Fuel Blends*, presented at 9th U. S. National Combustion Meeting Organized by the Central States Section of the Combustion Institute, May 17-20, 2015, Cincinnati, Ohio.

P. C. Ma, M. B. Nik, S. E. Carbajal, M. Ihme, T. Buschhagen, S. V. Naik, J. P. Gore, R. P. Lucht, "Large-Eddy Simulations of Fuel Injection and Atomization of a Hybrid Air-Blast Atomizer." To be presented at AIAA SciTech Meeting, San Diego, January 2015.

References

[1] Constantinou, L., and Rafiqul G. "New group contribution method for estimating properties of pure compounds." *AIChE Journal* 40.10 (1994): 1697-1710.

[2] Burger, M., Schmehl, R., Prommersberger, K., Schäfer, O., Koch, R., & Wittig, S. (2003). Droplet evaporation modeling by the distillation curve model: accounting for kerosene fuel and elevated pressures. *International journal of heat and mass transfer*, 46(23), 4403-4412.

[3] Lippert, A. M., & Reitz, R. D. (1997). *Modeling of multicomponent fuels using continuous distributions with application to droplet evaporation and sprays* (No. 972882). SAE Technical Paper.



- [4] Joback, K. G., & Reid, R. C. (1987). Estimation of pure-component properties from group- contributions. *Chemical Engineering Communications*, 57(1-6), 233-243.
- [5] Hansen, H. K., Rasmussen, P., Fredenslund, A., Schiller, M., & Gmehling, J. (1991). Vapor- liquid equilibria by UNIFAC group contribution. 5. Revision and extension. *Industrial & Engineering Chemistry Research*, 30(10), 2352-2355.
- [6] Sazhin, Sergei. *Droplets and sprays*. Springer, 2014.
- [7] Ranz, W. E., & Marshall, W. R. (1952). Evaporation from drops. *Chem. Eng. Prog*, 48(3), 141-146.
- [8] Wilke, C. R., & Lee, C. Y. (1955). Estimation of diffusion coefficients for gases and vapors. *Industrial & Engineering Chemistry*, 47(6), 1253-1257.
- [9] Neufeld, P. D., Janzen, A. R., & Aziz, R. A. (1972). Empirical Equations to Calculate 16 of the Transport Collision Integrals Ω (l, s)* for the Lennard-Jones (12-6) Potential. *The Journal of Chemical Physics*, 57(3), 1100-1102.
- [10] Yamada, T., & Gunn, R. D. (1973). Saturated liquid molar volumes. Rackett equation. *Journal of Chemical and Engineering Data*, 18(2), 234-236.
- [11] Elwardany, A. E., & Sazhin, S. S. (2012). A quasi-discrete model for droplet heating and evaporation: application to Diesel and gasoline fuels. *Fuel*, 97, 685-694.
- [12] Edwards, T., Moses, C., & Dryer, F. (2010, July). Evaluation of combustion performance of alternative aviation fuels. In *Nashville, 46th AIAA/ASME/SAE/ASEE Joint Propulsion Conference & Exhibit, AIAA-2010-7155*.
- [13] Magnussen, T., Rasmussen, P., & Fredenslund, A. (1981). UNIFAC parameter table for prediction of liquid-liquid equilibria. *Industrial & Engineering Chemistry Process Design and Development*, 20(2), 331-339.
- [14] Lee, B. I., & Kesler, M. G. (1975). A generalized thermodynamic correlation based on three- parameter corresponding states. *AIChE Journal*, 21(3), 510-527.
- [15] Ra, Y., & Reitz, R. D. (2009). A vaporization model for discrete multi-component fuel sprays. *International Journal of Multiphase Flow*, 35(2), 101-117.
- [16] Dooley, S., Won, S. H., Haas, F. M., Santner, J., Ju, Y., Dryer, F. L., & Farouk, T. I. Development of Reduced Kinetic Models for Petroleum-Derived and Alternative Jet Fuels.