# An Error Quantification of the Arrhenius Blending Rule for Viscosity of Hydrocarbon Mixtures

Randall C. Boehm[a,*], Franchesca Hauck[a], Zhibin Yang[a], C. Taber Wanstall[a], Joshua S. Heyne[a]

[a]*University of Dayton, 300 College Park, Dayton, OH 45469-0238, USA*
[*]Email: rboehm1@udayton.edu

**Definitions of the following terms: nearest neighbor, vacancy, relaxed state, perturbed state, molecular-scale-mixing, and cluster-scale-mixing.**

**A nearest neighbor** is defined here as each of the 12 lattice sites that surrounds a central lattice site in the ccp packing arrangement. The distance ($D_n$) between two lattice sites is derived from the molar volume ($\overline{V_{sol}}$) of the corresponding solid state of the components (A and B) that comprise the liquid, plus an arbitrary scalar of 1.5. This derivation is expressed by Equation 3.

$$D_n = 1.5 * 1.47 * 10^{-8} * (x_A * \sqrt[3]{\overline{V_{sol,A}}} + x_B * \sqrt[3]{\overline{V_{sol,B}}}) \quad (3)$$

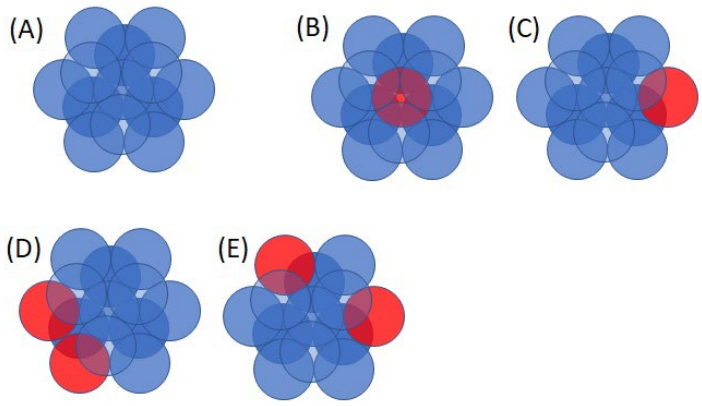


Figure 1: Nearest Neighbor and Vacancy Definitions. A) A central molecule with 12 homogeneous neighbors. B) A central vacancy surrounded by 12 neighboring molecules. C) A central molecule with 11 homogeneous neighbors and 1 neighboring vacancy. D) A central molecule with 10 homogeneous neighbors and 2 neighboring, adjacent vacancies. E) A central molecule with 10 homogeneous neighbors and 2 neighboring vacancies.

**A vacancy** is defined as a lattice site that is not occupied by molecule. This is further clarified by Figure 1.

**The relaxed state** is defined as a spatial arrangement of molecules and vacancies within a control volume that minimizes the sum of the pairwise interaction potentials, applicable to another control volume that is completely inscribed within the original control volume, and subject to the constraint that vacancies are probabilistically distributed throughout the original control volume and in sufficient concentration to account for the molar volume difference between the liquid and solid states of the components.

**The perturbed state** is defined as a spatial arrangement of molecules and vacancies within a control volume such that a single, central molecule is halfway between two adjacent lattice sites and single vacancy is split between the two adjacent lattice sites. This is further clarified by Figure 2. The significance of the dashed, solid, or colored borders in the exploded view will be discussed later.

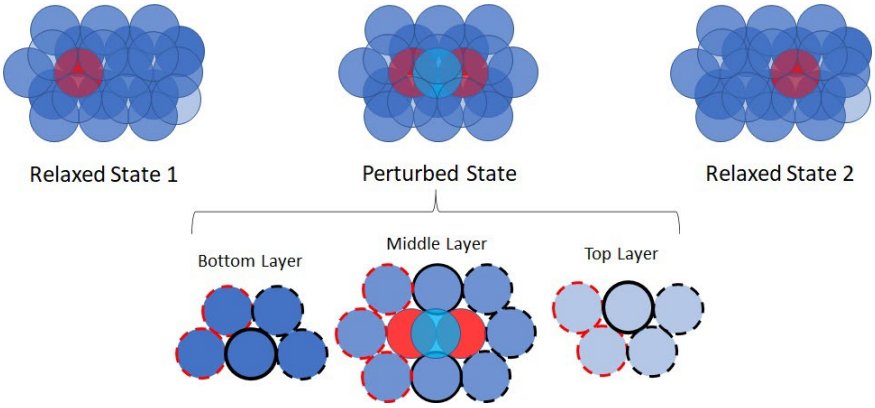


Figure 2: Perturbed state definition. Analogous to a transition state in chemical reactions. The perturbed state in this example corresponds to the midpoint as the central molecule travels from right to left between two lattice sites. In the exploded view, molecules that are being approached by the traveling molecule are denoted by a dashed red border. Molecules that are being distanced by the traveling molecule are denoted by a dashed black border. Molecules that that need to be pushed out of the way by the traveling molecule are denoted by a solid black border.

**Molecular-scale-mixing** implies that the occupancy (component A, component B, or vacancy) of each lattice site of the liquid's structure is determined probabilistically, weighted by the relative proportions of each potential occupant.

**Cluster-scale-mixing** implies that the occupancy (component A, component B, or vacancy) of each lattice site of the liquid's structure is not determined probabilistically. Rather, most of the nearest neighbor interactions are homogeneous.