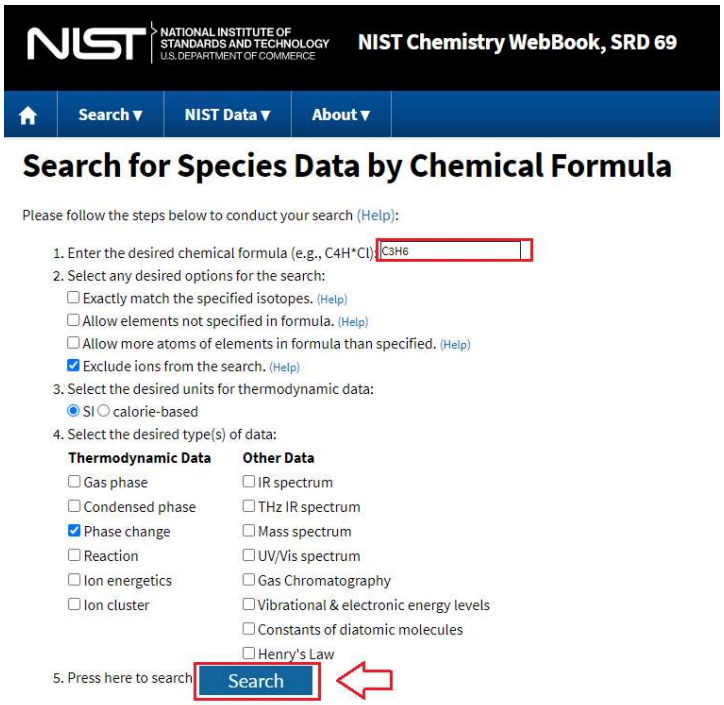
Preparing input data for real-fluid calculations in OpenFOAM

by Danh Nam Nguyen

```
dataForRealFluid    // of Oxygen species
{
    Tc      154.58;  // the critical temperature, K
    Pc      5.043;   // the critical pressure, MPa
    Vc      73.529;  // the critical volume, cm^3/mol
    omega   0.025;   // the dimensionless acentric factor
    kappai  0.0;     // the dimensionless association factor
    miui    0.0;     // the dimensionless dipole moment
    sigmvi  16.6;    // the dimensionless diffusion volume
}
```

1. critical data table (including Tc [K], Pc [MPa], Vc [cm3/mol], acentric factor [-])

These values can be found from the NIST database https://webbook.nist.gov/chemistry/form-ser/



In case (for instance, intermediate species) you only find these values (Tc, Pc, Vc), the following relation can be used: (referred from CHERIC, chemical engineering and materials information center https://www.cheric.org/)

$$v_c = 3.29\sigma^3 \pm 0.07$$
$$T_c = (1.316 \pm 0.006)\frac{\varepsilon}{k}$$
$$p_c = 0.08864\frac{RT_c}{mb_i} = \frac{0.08864}{0.873}\frac{RT_c}{N\sigma^3} = 1.4 \times 10^{-24}\frac{T_c}{\sigma^3}$$

where the value of ε/k and σ can be taken from Trans.dat file in CHEMKIN format.

5.3. Transport Data Included with CHEMKIN

Table 5.1: Species in *Transport* Database (p. 88) lists the species contained in the ANSYS Chemkin-Pro tran.dat file, which is included in every installation, as the corresponding data for each species.

Table 5.1: Species in *Transport* Database

Species Name	Geometry	ε/k_B	σ	μ	α	Z_{rot}
Al2Me6	2	471.	6.71	0.0	0.0	1.0
AlMe3	2	471.	5.30	0.0	0.0	1.0
AR	0	136.500	3.330	0.000	0.000	0.000
AR*	0	136.500	3.330	0.000	0.000	0.000

You can also refer to CriticalConstants.pdf file (provided along with this file) for finding acentric factor and critical data that can not be found in the NIST database.

2. Transport data table (including kappai, miui, sigmvi)

2.1. kappai

This is the dimensionless association factor, from Table 9.1 (referred to the textbook of Poling et al.).

Refer to Chung et al. (1998) we have more data:

Table I. Association Parameters

compd	κ	compd	κ
methanol	0.215 175	1-pentanol	0.121 555
ethanol	0.174 823	1-hexanol	0.114 230
1-propanol	0.143 453	1-heptanol	0.108 674
2-propanol	0.143 453	acetic acid	0.091 549
1-butanol	0.131 671	water	0.075 908
2-methyl-1-propanol	0.131 671		

For other alcohols not shown in Table 9-1, this value can be evaluated by equation (see the highlighted text).

In Eq. (9-4.11), ω is the acentric factor (See Chap. 2) and κ is a special correction for highly polar substances such as alcohols and acids. Values of κ for a few such materials are shown in Table 9-1. Chung, et al. (1984) suggest that for other alcohols not shown in Table 9-1, $\kappa = 0.0682 + 4.704$[(number of –OH groups)/molecular weight]. The term μ_r is a dimensionless dipole moment. (See discussion in Chap. 2 and also under Eq. (9-4.17) for techniques to nondimensionalize a dipole moment.) When V_c is in cm³/mole, T_c is in kelvins, and μ is in debyes,

For non-alcoholic species, this value is zero.

2.2. miui (dipole moment)

This is μ, dipole moment in debyes (it's not dimensionless dipole moment, I made a mistake in Listing 2 in my paper Nguyen et al. CPC 273 (2022) 108264), taken from Trans.dat file in CHEMKIN format.

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AS	0	1045.5	4.580	0.000	0.000	0.000
AS2	1	1045.5	5.510	0.000	0.000	1.000
ASH	1	199.3	4.215	0.000	0.000	1.000

2.3. sigmvi (dimensionless diffusion volume)

This can be found from the NIST database for specific species. If there is no data available in the NIST database, you can calculate this value based one the atomic diffusion volume as:

3. sigmvi (diffusion volume)	H	C	O	N
atomic diffusion volume	1.98	16.5	5.48	5.69

Then, the diffusion volume of a species CxHyOzNn is:

$$sigmvi = n_C sigmvi_C + n_H sigmvi_H + n_O sigmvi_O + n_N sigmvi_N$$

Or

$$sigmvi = x * 16.5 + y * 1.98 + z * 5.48 + n * 5.69$$

For example, $sigmvi_{CH4} = 24.42$

You can refer to some excel files that I made (provided along with this file) for several chemical mechanisms.

Finally, to make the *thermos.inputData* for real-fluid in OF format, you can generate the *thermos.inputData* for ideal gas model first by running *chemkinToFoam* utility. Then, update these values for real-fluid model manually. I will write a utility in OF to generate this file for real-fluid models in the future.

Enjoy.