NREL/TP-425-20685 • UC Category: 1503 • DE96007902

Development of an ASPEN PLUS Physical Property Database for Biofuels Components

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A national laboratory of
the U.S. Department of Energy
Managed by Midwest Research Institute
for the U.S. Department of Energy
under Contract No. DE-AC36-83CH10093

Prepared under Task No. BF521004

April 1996

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Introduction

Physical property data for many of the key components used in the simulation for the ethanol from lignocellulose process are not available in the standard ASPEN PLUS property databases. Indeed, many of the properties necessary to successfully simulate this process are not available anywhere. In addition, inputting the available properties into each simulation is awkward and tedious, and mistakes can be easily introduced when a long list of physical property equation parameters is entered. Therefore, we must evaluate the literature, estimate properties where necessary, and determine a set of consistent physical properties for all components of interest. The components must then be entered into an in-house NREL ASPEN PLUS database so they can be called on without being retyped into each specific simulation.

The first phase of this work is complete. A complete set of properties for the currently identifiable important compounds in the ethanol process is attached. With this as the starting base we can continue to search for and evaluate new properties or have properties measured in the laboratory and update the central database.

Aspen's Approach to Physical Properties

The Aspen simulator handles three classes of compounds:

1. Those (such as ethanol) that are involved in vapor liquid equilibrium;

2. Those (such as $CaSO_4$) that are solids only and are identifiable; and

3. Solids (such as coal) that are identifiable by attribute only.

This database will deal with the first two types only.

For compounds involved in vapor liquid equilibrium, the simulator must have a complete set of properties to allow it to do flash calculations, even though the compound may be a very high boiler and will stay in the liquid phase exclusively. Also, materials such as glucose and xylose, which are commonly solids but will be used exclusively in aqueous solution in the process, will be treated as liquids.

The second class, which includes cellulose and gypsum, is assumed to comprise conventional solids whose properties requirements are very minimal. A conventional solid can (unlike nonconventional solids that must be described by attributes) be defined by a chemical formula.

Minimum Physical Properties Required by Aspen

The minimum physical properties required by Aspen depend on the calculation routes selected for fundamental properties such as liquid, vapor, and solid enthalpy and density. In general, because of the need to distill ethanol and to handle dissolved gases, the standard NRTL (non-random two liquid or Renon) route is used. This route, which includes the NRTL liquid activity coefficient model, Henry's law for the dissolved gases, and RKS (Redlich-Kwong-Soave) equation of state for the vapor phase, is used to calculate properties for components in the liquid and vapor phases. It also uses the Ideal Gas (IG) at 25°C as the standard reference state, thus requiring the heat of formation at these conditions (Table 1).

Table 1. Required Properties

Liquids/Gases	Conventional Solids
Critical Temperature	Heat of Formation
Critical Pressure	Heat Capacity
IG Heat of Formation @ 298.15K	Density
Vapor Pressure	
IG Heat Capacity	
Heat of Vaporization	
Liquid Density	

Many components used here will not be involved in vapor liquid equilibrium, as they stay in the liquid phase under the operating conditions experienced during the ethanol process. However, because of the above requirements, vapor properties will be needed. These will be estimated, but as long as the vapor pressure is low enough, the compounds will never actually show up in the vapor phase, and the liquid properties of interest will be calculated correctly.

Table 2 lists the compounds included in the current database, along with their primary state and formula. Isomers were not considered independently; because most of the desired properties are being estimated, there will not be a significant difference between isomers. This will not preclude the use of isomers in simulations, but there will be no physical difference between isomers in the simulations. For example, all five-carbon sugars should use the properties of xylose, and six-carbon sugars those of glucose. The chemical formulas used for compounds such as biomass and cellulase were obtained from Radian Corporation[1] and Putsche,[2] respectively. Solslds are essentially everything combustible that is not one of the identifiable cellulose, lignin, or hemicellulose materials in biomass. The formula for solslds corresponds to the difference between the ultimate analysis of the biomass and the number of identifiable compounds. The heating value of solslds is the difference between that of the original biomass and the sum of the identifiable components. The solslds listed here correspond to poplar biomass and would differ for other sources of biomass. The solunkn is a compound that elutes at a similar position to xylitol, but is unknown. It was given a reduced formula of xylose for material balances only.

Table 2. Compounds Included in the ASPEN PLUS Database (INHSPCD)

Compound Name	Formula	Database Name	Database Alias	Normal State
Glucose	$C_6H_{12}O_6$	GLUCOSE	C6H12O6	Liquid (aqueous)
Xylose	$C_5H_{10}O_5$	XYLOSE	C5H10O5	Liquid (aqueous)
Cellulose	$C_6H_{10}O_5$*	CELLULOS	C6H10O5	Solid
Xylan	$C_5H_8O_4$-	XYLAN	C5H8O4	Solid
Lignin	$C_{7.3}H_{13.9}O_{1.3}$	LIGNIN	CXHXOX	Solid
Biomass (cell mass)	$CH_{1.64}N_{0.23}O_{0.39}S_{0.0035}$	BIOMASS	CHXNXOXSX-1	Solid
Cellulase	$CH_{1.57}N_{0.29}O_{0.31}S_{0.007}$	CELLULAS	CHXNXOXSX-2	Solid
Zymo	$CH_{1.8}O_{0.5}N_{0.2}$	ZYMO	CHXOXNX	Solid
Solslds	$CH_{1.48}O_{0.019}S_{0.0013}$	SOLSLDS	CHXOXSX	Liquid (aqueous)
Solunkn	$C_{0.5}HO_{0.5}$	SOLUNKN	CXHOX	Liquid (aqueous)
Gypsum	$CaSO_4 \cdot 2H_2O$	GYPSUM	CaSO4-2H2O	Solid

* For the polymeric compounds a formula corresponding to a single repeat unit was used.

Combustion Stoichiometry

In all cases the heat of combustion was found in the literature or estimated and used to calculate the heat of formation. To calculate the heat of formation necessary for other heat of reaction calculations, we must know the compound's molecular formula (and consequently its combustion stoichiometry). Given the above molecular formulas, the combustion stoichiometry used for each compound is given below.

Glucose
$C_6H_{12}O_6 + 6\ O_2 \rightarrow 6\ H_2O + 6\ CO_2$ M

Xylose
$C_5H_{10}O_5 + 5\ O_2 \rightarrow 5\ H_2O + 5\ CO_2$ M

Cellulose
$C_6H_{10}O_5 + 6\ O_2 \rightarrow 5\ H_2O + 6\ CO_2$

Xylan
$C_5H_8O_4 + 5\ O_2 \rightarrow 4\ H_2O + 5\ CO_2$ M

Lignin
$C_{7.3}H_{13.9}O_{1.3} + 10.125\ O_2 \rightarrow 6.95\ H_2O + 7.3\ CO_2$

Biomass
$CH_{1.64}N_{0.23}O_{0.39}S_{0.0035} + 1.2185\ O_2 \rightarrow 0.82\ H_2O + CO_2 + 0.0035\ SO_2 + 0.115\ N_2$

Cellulase
$CH_{1.57}N_{0.29}O_{0.31}S_{0.007} + 1.2445\ O_2 \rightarrow 0.785\ H_2O + CO_2 + 0.007\ SO_2 + 0.145\ N_2$

Zymo
$CH_{1.8}O_{0.5}N_{0.2} + 1.2\ O_2 \rightarrow 0.9\ H_2O + CO_2 + 0.1\ N_2$

Solslds
$CH_{1.48}O_{0.19}S_{0.0013} + 1.2763\ O_2 \rightarrow 0.74\ H_2O + CO_2 + 0.0013\ SO_2$

Solunkn
$C_{0.5}HO_{0.5} + 0.5\ O_2 \rightarrow 0.5\ H_2O + 0.5\ CO_2$

In addition to the reaction stoichiometry, the heat of formation of the combustion products is required to calculate heat of formation from heat of combustion. The values used here are:

Compound	Heat of Formation @ 298 K	
H_2O (liquid)	-68.7979 kcal/mole	-2.88043×10^8 J/Kmole
CO_2 (IG)	-94.052 kcal/mole	-3.93776×10^8 J/Kmole
SO_2 (IG)	-70.899 kcal/mole	-2.9684×10^8 J/Kmole

These values were taken from the ASPEN PLUS Pure Component databank to be consistent with the calculations to be performed in ASPEN PLUS.

Description of Properties Included in the Database

Following is a description of the source methods and estimation used to develop properties for all compounds listed above. These properties are in the new ASPEN PLUS INHSPCD (Inhouse Pure Component Database) and are enclosed as inputs to the DFMS (Data File Management System) (Appendix A) and as ASPEN PLUS Input language PROP-DATA statements (Appendix B). (All properties are in SI units.) A summary of sources of all properties appears in Appendix C and a summary of the properties in the in-house database appears in Appendix D.

The ASPEN PLUS DFMS allows a source code to be entered for each property. Rather than using an actual reference number, this is used for a quality code. The following quality codes have been assigned to each data set. In general, data with a higher confidence level correspond to higher numbers.

Data Quality Codes Used in the Biofuels INHSPCD

Code	Code Description
9	Literature data
8	Regressed to literature data
7	Calculated directly (e.g. MW)
6	Calculated from other literature data (e.g. ΔH_F° H_{COMB})
5	Estimated from the commercial property estimation package PREDICT
4	Estimated, but not from PREDICT
3	Copied literature data from a similar compound on a mass basis
2	Copied literature data from a similar compound on a mole basis
1	Copied data of various origin from a similar compound
0	Unknown origin

Glucose

Glucose, although a generally considered a solid at the temperatures involved in the ethanol process, is exclusively in aqueous solution. It will therefore be modeled as a liquid, although it will never exist as a pure liquid in the process. The properties listed here are NOT intended for use with pure glucose, or even with concentrated solutions. The vapor pressure is low enough (the normal boiling point has been estimated to be higher than 800 K) that the glucose will never be flashed into the vapor stream.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Critical Temperature	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Critical Pressure	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Critical Volume	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Acentric Factor	(5)	Estimated using the Pitzer[4] vapor pressure correlation and the estimated normal boiling point in PREDICT.
IG Heat of Formation	(6)	Literature[5] value was -1.2735x10^9 J/Kmole. Using this value, and the ΔH_F(liquid) calculated from the literature value for higher ΔH_C (673 kcal/mole[4]), the heat of vaporization (difference between ΔH_F [IG] and ΔH_F [liquid or solid, ΔH_{SOLN} is small]) would have to be less than zero. Therefore, the heat of vaporization was set at a very small value (see below) and the ΔH_F(IG) from the literature adjusted slightly to give the value of -1.2569x10^9 J/Kmole used in the database. See Table 3 for a comparison of the original ΔH_C and those back calculated from Aspen.
IG Free Ergy. of Form. @ 298.15 K	(9)	Literature[5]

Table 3. High Heating Values (Heat of Combustion) Comparison of ASPEN Calculated Values and Literature									
		Higher Heating Values Calculated from ASPEN				Higher Heating Values Calculated from Literature			
	MW	J/Kmol	Kcal/gmole	BTU/lbmole	BTU/lb	J/Kmol	Kcal/gmole	BTU/lbmole	BTU/l
Glucose	180.16	2.81776E+09	673.01	1212242	6728.70		673		
Xylose	150.132	2.35178E+09	561.71	1011771	6739.21		561.5		
Cellulose	162.1436	2.81312E+09	671.90	1210246	7464.04	2.81311E+09	671.8987	1210240	7464
Xylan	132.117	2.34787E+09	560.78	1010089	7645.41		560.6		
Lignin	122.493	3.26548E+09	779.95	1404858	11468.88	3.26751E+09	780.4304	1405730	11476
Biomass	23.238	5.31676E+08	126.99	228734.9	9843.14	5.32425E+08	127.1674	229057	9857
Zymo	24.6264	5.20125E+08	124.23	223765.5	9086.41		124.8		
Cellulase	22.8398	5.44906E+08	130.15	234426.7	10263.95	5.45015E+08	130.1745	234473.4	10266
Solslds	16.5844	5.53575E+08	132.22	238156.2	14360.25		132.7		
Solunkn	15.0134	2.16411E+08	51.69	93103.23	6201.34		52		
EtOH	46.0691	1.36661E+09	326.41	587935.9	12762.04		327.6		
Heat of Reaction to Form Ethanol Calculated from ASPEN						Heat of Rxn to Form EtOH from Literature			
Glucose	180.16	8.45388E+07	20.19	36369.85	201.88		19.6		
Xylose	150.132	7.41032E+07	17.70	31880.3	212.35		15.5		

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Vapor Pressure	(5)	Estimated using the Pitzer[4] corresponding states method with the above critical properties and fit to the ASPEN PLUS PLXANT extended Antoine model.
IG Heat Capacity	(6)	Used a constant value for solid glucose at 20°C from the literature[6] and assumed it was the same as the liquid heat capacity. Using the heat of vaporization listed below, a single parameter in this equation was adjusted to the match the liquid heat capacity.
Heat of Vaporization	(0)	Set to an arbitrarily low value of 0.12 kcal/mole (5.02×10^5 J/Kmole) at 298 K. The standard exponent for the Watson[7] equation of 0.38 was used with the set value at 298 K in the Aspen DHVLWT (Watson) correlation.
Liquid Density	(8)	The Aspen single parameter in the Rackett[8] was regressed using literature[6] data for glucose water solutions and water data from the Aspen PURECOMP database. The results of this regression are given in Table 4.
Liquid Heat Capacity	(9)	Used a constant value for solid glucose at 20°C from the literature[6].

Table 4. Glucose/Water Solution Density at 20°C, Regression to the ASPEN PLUS Rackett Equation											
Mole Frac H2O	Density Data g/cc	Density Estimated g/cc	Std-Dev	Absolute Diff.	Percent Diff.	Mole Frac H2O	Density Data g/cc	Density Estimated g/cc	Std-Dev	Absolute Diff.	Percent Diff.
0.9995	1.0001	1.00023	1.00E-02	1.32E-04	1.32E-02	0.9813	1.0624	1.06365	1.06E-02	1.25E-03	0.11747
0.99899	1.002	1.00215	1.00E-02	1.52E-04	1.52E-02	0.9799	1.0667	1.06801	1.07E-02	1.31E-03	0.12319
0.99848	1.0039	1.00408	1.00E-02	1.78E-04	1.78E-02	0.9785	1.071	1.07241	1.07E-02	1.41E-03	0.13199
0.99796	1.0058	1.00602	1.01E-02	2.18E-04	2.17E-02	0.9770	1.0753	1.07684	1.08E-02	1.54E-03	0.14352
0.99744	1.0078	1.00796	1.01E-02	1.59E-04	1.58E-02	0.9756	1.0797	1.08131	1.08E-02	1.61E-03	0.149
0.99692	1.0097	1.00991	1.01E-02	2.13E-04	2.11E-02	0.9725	1.0884	1.09033	1.09E-02	1.93E-03	0.17694
0.99639	1.0116	1.01188	1.01E-02	2.76E-04	2.73E-02	0.9693	1.0973	1.09946	1.10E-02	2.16E-03	0.1969
0.99585	1.0136	1.01384	1.01E-02	2.44E-04	2.41E-02	0.9660	1.1063	1.10871	1.11E-02	2.41E-03	0.21817
0.99531	1.0155	1.01582	1.02E-02	3.24E-04	3.19E-02	0.9625	1.1154	1.11807	1.12E-02	2.67E-03	0.23943
0.99477	1.0175	1.01781	1.02E-02	3.08E-04	3.03E-02	0.9589	1.1246	1.12753	1.12E-02	2.93E-03	0.26046
0.99421	1.0194	1.0198	1.02E-02	4.04E-04	3.96E-02	0.9550	1.134	1.13708	1.13E-02	3.08E-03	0.27137
0.99366	1.0214	1.02181	1.02E-02	4.07E-04	3.99E-02	0.9510	1.1434	1.1467	1.14E-02	3.30E-03	0.28886
0.9931	1.0234	1.02382	1.02E-02	4.21E-04	4.12E-02	0.9467	1.1529	1.1564	1.15E-02	3.50E-03	0.3032
0.99253	1.0254	1.02584	1.03E-02	4.39E-04	4.28E-02	0.9422	1.1626	1.16614	1.16E-02	3.54E-03	0.30437
0.99196	1.0274	1.02787	1.03E-02	4.71E-04	4.58E-02	0.9375	1.1724	1.17592	1.17E-02	3.52E-03	0.29985
0.99138	1.0294	1.02991	1.03E-02	5.05E-04	4.91E-02	0.9324	1.1823	1.18571	1.18E-02	3.41E-03	0.28804
0.9908	1.0314	1.03195	1.03E-02	5.53E-04	5.37E-02	0.9271	1.1924	1.19549	1.19E-02	3.09E-03	0.25884
0.99021	1.0334	1.03401	1.03E-02	6.07E-04	5.88E-02	0.9215	1.2026	1.20523	1.20E-02	2.63E-03	0.21854
0.98961	1.0354	1.03607	1.04E-02	6.70E-04	6.47E-02	0.9155	1.213	1.2149	1.21E-02	1.90E-03	0.15688
0.98901	1.0375	1.03814	1.04E-02	6.42E-04	6.19E-02	0.9090	1.2235	1.22447	1.22E-02	9.73E-04	7.95E-
0.98779	1.0416	1.04231	1.04E-02	7.08E-04	6.79E-02	0.9022	1.2342	1.2339	1.23E-02	-3.04E-	-2.46E-
0.98655	1.0457	1.04651	1.05E-02	8.12E-04	7.76E-02	0.8949	1.2451	1.24313	1.25E-02	-1.98E-	-0.15863
0.98528	1.0498	1.05074	1.05E-02	9.44E-04	9.00E-02	0.8871	1.2562	1.25211	1.26E-02	-4.09E-	-0.32591
0.98398	1.054	1.05501	1.05E-02	1.01E-03	9.61E-02	0.8786	1.2676	1.26077	1.27E-02	-6.83E-	-0.53851
0.98266	1.0582	1.05932	1.06E-02	1.12E-03	0.10542	0.8695	1.2793	1.26905	1.28E-02	-1.02E-	-0.80095
ROOT MEAN SQUARE DEVIATION = 0.2490574E-02											
AVERAGE DEVIATION = 0.7325108E-03											
AVERAGE ABSOLUTE DEVIATION = 0.1670345E-02											
MAXIMUM DEVIATION = -0.1024660E-01											
RMS RELATIVE DEVIATION = 0.2061817E-02											
AVG. ABS. REL. DEVIATION = 0.1445592E-02											

Xylose

Xylose, like glucose, is a generally considered a solid at the temperatures involved in the ethanol process, but is exclusively in aqueous solution. Therefore, it will be modeled as a liquid, although it will never exist as a pure liquid in the process. The properties listed here are NOT intended for use with pure xylose or even with concentrated solutions. The vapor pressure is low enough (the normal boiling point has been estimated to be higher than 800 K) that the xylose will never be flashed into the vapor stream.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Critical Temperature	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Critical Pressure	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Critical Volume	(5)	Estimated using the Joback[3] group contribution method in PREDICT.
Acentric Factor	(5)	Estimated using the Pitzer[4] vapor pressure correlation and the estimated normal boiling point in PREDICT.
IG Heat of Formation @ 298.15 K	(6)	As with glucose, the heat of vaporization was set at an arbitrarily low value and the ΔH_F (IG) was back calculated using that heat of M vaporization and the literature value of heat of combustion (561.5 Kcal/mole[6]). See Table 3 for a comparison of the original ΔH_C and M that back calculated from Aspen.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Vapor Pressure	(5)	Estimated using the Pitzer[4] corresponding states method with the above critical properties and fit to the Aspen+ PLXANT extended Antoine model.
IG Heat Capacity	(3)	Used a constant value for solid glucose at 20°C from the literature[6] and assumed it was the same as the liquid heat capacity. Using the heat of vaporization listed below, a single parameter in this equation was adjusted to the match the liquid heat capacity.
Heat of Vaporization	(0)	Set to an arbitrarily low value of 1 Kcal/mole (4.1868×10^6) at 298 K. The standard exponent for the Watson[7] equation of 0.38 was used with the set value at 298 K in the Aspen DHVLWT (Watson) correlation.
Liquid Density	(3)	The Aspen single parameter in the Rackett[8] was regressed using the literature[9] data for glucose water solutions on a mass basis (g/L) and water data from the Aspen PURECOMP database. The results of this regression are given in Table 5.
Liquid Heat Capacity	(3)	Used a constant value for solid glucose at 20°C from the literature[6].

Table 5. Xylose/Water Solution Density at 20°C, Regression to the ASPEN PLUS Rackett Equation Using Glucose/Water Mass Basis, Converted to Xylose/Water on a Mole Basis

Mole Frac H2O	Density Data g/cc	Density Estimate g/cc	Std-Dev	Absolute Diff.	Percent Diff.	Mole Frac H2O	Density Data g/cc	Density Estimated g/cc	Std-Dev	Absolute Diff.	Percent Diff.
0.9995	1.0001	1.00001	1.00E-02	-8.63E-05	-8.63E-03	0.98131	1.0624	1.05752	1.06E-02	-4.88E-03	-0.45941
0.99899	1.002	1.00172	1.00E-02	-2.84E-04	-2.83E-02	0.97993	1.0667	1.06159	1.07E-02	-5.11E-03	-0.47887
0.99848	1.0039	1.00343	1.00E-02	-4.74E-04	-4.72E-02	0.97852	1.071	1.06571	1.07E-02	-5.29E-03	-0.49362
0.99796	1.0058	1.00515	1.01E-02	-6.50E-04	-6.46E-02	0.97708	1.0753	1.06988	1.08E-02	-5.42E-03	-0.50394
0.99744	1.0078	1.00688	1.01E-02	-9.22E-04	-9.15E-02	0.97561	1.0797	1.0741	1.08E-02	-5.60E-03	-0.51848
0.99692	1.0097	1.00862	1.01E-02	-1.08E-03	-0.10706	0.97257	1.0884	1.08269	1.09E-02	-5.71E-03	-0.52493
0.99639	1.0116	1.01037	1.01E-02	-1.23E-03	-0.12154	0.96939	1.0973	1.09147	1.10E-02	-5.83E-03	-0.53108
0.99585	1.0136	1.01213	1.01E-02	-1.47E-03	-0.14515	0.96606	1.1063	1.10047	1.11E-02	-5.83E-03	-0.52699
0.99531	1.0155	1.0139	1.02E-02	-1.60E-03	-0.15755	0.96257	1.1154	1.10968	1.12E-02	-5.72E-03	-0.51315
0.99477	1.0175	1.01568	1.02E-02	-1.82E-03	-0.17908	0.95891	1.1246	1.1191	1.12E-02	-5.50E-03	-0.48891
0.99421	1.0194	1.01747	1.02E-02	-1.93E-03	-0.18948	0.95506	1.134	1.12875	1.13E-02	-5.25E-03	-0.46317
0.99366	1.0214	1.01927	1.02E-02	-2.13E-03	-0.20869	0.95101	1.1434	1.13862	1.14E-02	-4.78E-03	-0.41832
0.9931	1.0234	1.02108	1.02E-02	-2.32E-03	-0.22661	0.94675	1.1529	1.14872	1.15E-02	-4.18E-03	-0.36294
0.99253	1.0254	1.0229	1.03E-02	-2.50E-03	-0.24389	0.94225	1.1626	1.15905	1.16E-02	-3.55E-03	-0.30577
0.99196	1.0274	1.02473	1.03E-02	-2.67E-03	-0.25962	0.9375	1.1724	1.16961	1.17E-02	-2.79E-03	-0.23814
0.99138	1.0294	1.02657	1.03E-02	-2.83E-03	-0.27476	0.93248	1.1823	1.18041	1.18E-02	-1.89E-03	-0.16019
0.9908	1.0314	1.02843	1.03E-02	-2.97E-03	-0.28839	0.92715	1.1924	1.19144	1.19E-02	-9.60E-04	-8.05E-
0.99021	1.0334	1.03029	1.03E-02	-3.11E-03	-0.30117	0.9215	1.2026	1.20271	1.20E-02	1.06E-04	8.81E-
0.98961	1.0354	1.03216	1.04E-02	-3.24E-03	-0.3128	0.9155	1.213	1.21421	1.21E-02	1.20E-03	9.93E-
0.98901	1.0375	1.03405	1.04E-02	-3.45E-03	-0.33292	0.90909	1.2235	1.22593	1.22E-02	2.43E-03	0.19859
0.98779	1.0416	1.03785	1.04E-02	-3.76E-03	-0.36054	0.90226	1.2342	1.23787	1.23E-02	3.67E-03	0.29769
0.98655	1.0457	1.04169	1.05E-02	-4.01E-03	-0.38333	0.89495	1.2451	1.25003	1.25E-02	4.93E-03	0.39573
0.98528	1.0498	1.04558	1.05E-02	-4.22E-03	-0.4021	0.8871	1.2562	1.26238	1.26E-02	6.18E-03	0.49187
0.98398	1.054	1.04951	1.05E-02	-4.49E-03	-0.42565	0.87866	1.2676	1.27491	1.27E-02	7.31E-03	0.57665
0.98266	1.0582	1.0535	1.06E-02	-4.71E-03	-0.44467	0.86957	1.2793	1.2876	1.28E-02	8.29E-03	0.64839

ROOT MEAN SQUARE DEVIATION	=	0.3947574E-02
AVERAGE DEVIATION	=	-0.2042724E-02
AVERAGE ABSOLUTE DEVIATION	=	0.3407739E-02
MAXIMUM DEVIATION	=	0.8294807E-02
RMS RELATIVE DEVIATION	=	0.3518716E-02
AVG. ABS. REL. DEVIATION	=	0.3078164E-02

Cellulose

Cellulose is considered to be a solid throughout the process and will never be in solution. Additionally, cellulose is a polymer, but its molecular weight formula will be taken as the repeat unit only. The other properties are determined on a weight basis and then converted to mole basis for the database, using the molecular weight of a repeat unit.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(6)	Using the a literature value for ΔH_c[10] the heat of formation was back calculated. See Table 3 for the original values of ΔH_c.

Temperature Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(9)	mass basis was used.
Solid Density	(3)	A literature value for starch[11] was used on a mass basis.

Xylan

Xylan is considered to be a solid throughout the process and will never be in solution. Additionally, xylan is a polymer, but its molecular weight formula will be taken as the repeat unit only. The other properties are determined on a weight basis and then converted to mole basis for the database, using the molecular weight of a repeat unit.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(2)	Assumed that the ratio of the ΔH_c of glucose to xylose would be the same as that for the ratio of cellulose to xylan. Using the glucose to xylose ΔH_c ratio and the ΔH_f from above for cellulose, the ΔH_f for xylan was approximated. From the ΔH_c, the heat of formation was calculated.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(3)	A literature polynomial[10] for cellulose from loblolly pine wood on a mass basis was used.
Solid Density	(3)	A literature value for starch[11] was used on a mass basis.

Lignin

Lignin is considered to be a solid throughout the process and will never be in solution.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(6)	Used ΔH_c value supplied by Riley[12] to calculate the heat of formation. M The ΔH_c of Riley is similar to a value given by the literature for soft-wood. The softwood literature[10] is 11340 BTU/# and the value from Riley is 11476 BTU/#.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(9)	Used literature value for polynomial[10].
Solid Density	(3)	Simply assume 1.5 g/cc (similar to starch).

Cellulase (Enzyme)

Cellulase is considered to be a solid throughout the process and will never be in solution.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(6)	Used ΔH_c value supplied by Putsche[2] to calculate heat of formation. Putsche calculated the ΔH_c using the approximation method of Bailey and Ollis[13].

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(4)	Estimated using Kopp's rule[6].
Solid Density	(3)	Simply assume 1.5 g/cc (similar to starch).

Biomass (Cell Mass)

Biomass is considered to be a solid throughout the process and will never be in solution.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(6)	Used ΔH_c value supplied by Putsche[2] to calculate heat of formation. Putsche calculated the ΔH_c using the approximation method of Bailey and Ollis[13].

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(4)	Estimated using Kopp's rule[6].
Solid Density	(3)	Simply assume 1.5 g/cc (similar to starch).

Zymo (Bacterium)

Zymo is considered to be a solid throughout the process and will never be in solution.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(4)	Estimated ΔH_c using a crude method of Bailey and Ollis[13] and then calculated the heat of formation.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(4)	Estimated using Kopp's rule[6].
Solid Density	(3)	Simply assume 1.5 g/cc (similar to starch).

Solslds (Soluble Solids)—Poplar Biomass

Solslds are the nonidentifiable solids that will be dissolved in aqueous solutions throughout the simulation. Therefore, they will never exist as a pure liquid in the process. The properties listed here are NOT intended for use with pure components, or even with concentrated solutions. The vapor pressure is low enough (the normal boiling point has been estimated to be higher than 800 K) such that the solslds will never be flashed into the vapor stream.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Critical Temperature	(1)	Used the value of glucose.
Critical Pressure	(1)	Used the value of glucose.
Critical Volume	(1)	Used the value of glucose.
Acentric Factor	(1)	Used the value of glucose.
IG Heat of Formation @ 298.15 K	(4)	ΔH_c value calculated to match the ΔH_c of poplar biomass and its identifiable components. This was verified using a crude method of Bailey and Ollis[13]. This value was then used to calculated the heat of formation of the liquid. A small value of 1 kcal/mole was assumed for the heat of vaporization and the IG heat of formation was calculated.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Vapor Pressure	(1)	Used the value of glucose.
IG Heat Capacity	(1)	Used a constant value for solid glucose at 20°C from the literature[6] and assumed it was the same as the liquid heat capacity. Using the heat of vaporization listed below, a single parameter in this equation was adjusted to the match the liquid heat capacity.
Heat of Vaporization	(0)	Assumed an arbitrary low value of 1 kcal/mole at 298 K.
Liquid Density	(0)	Assuming a value of water (1 g/cc) the Rackett parameter was back calculated using the above critical properties and molecular weight.
Liquid Heat Capacity	(3)	Used value for glucose on a mass basis.

Solunkn (Unknown Soluble Solids)

Solunkn is an unknown compound similar to xylose that will be dissolved in aqueous solutions through- out the simulation. Therefore, it will never exist as a pure liquid in the process. The properties listed here are NOT intended for use with pure compounds or even with concentrated solutions. The vapor pressure is sufficiently low (the normal boiling point has been estimated to be higher than 800 K) such that the solunkn will never be flashed into the vapor stream.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Critical Temperature	(1)	Used the value of xylose.
Critical Pressure	(1)	Used the value of xylose.
Critical Volume	(1)	Used the value of xylose.
Acentric Factor	(1)	Used the value of xylose.
IG Heat of Formation @ 298.15 K	(4)	Estimated ΔH_c using a crude method of Bailey and Ollis[13] and then calculated the heat of formation of the liquid. A small value of 1 kcal/mole was assumed for the heat of vaporization and the IG heat of formation was calculated.

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Vapor Pressure	(1)	Used the value of glucose.
IG Heat Capacity	(1)	Used a constant value for solid glucose at 20°C from the literature[6] and assumed it was the same as the liquid heat capacity. Using the heat of vaporization listed below, a single parameter in this equation was adjusted to match the liquid heat capacity.
Heat of Vaporization	(0)	Assumed an arbitrary low value of 1 kcal/mole at 298 K.
Liquid Density	(0)	Assuming a value of water (1 g/cc) the Rackett parameter was back calculated using the above critical properties and molecular weight.
Liquid Heat Capacity	(3)	Used value for glucose on a mass basis.

Gypsum

Gypsum is considered to be a solid throughout the process and will never be in solution.

Point Properties

Properties	(Quality Code)	Methodology
Molecular Weight	(7)	Calculated directly.
Solid Heat of Formation @ 298.15 K	(9)	Literature value[14].
Solid Free Energy of Formation @ 298.15 K	(9)	Literature value[14].

Temperature-Correlated Properties

Properties	(Quality Code)	Methodology
Solid Heat Capacity	(2)	Used literature value for $CaSO_4$[14].
Solid Density	(9)	Literature value[14].

Acknowledgment

This work was funded by the Biochemical Conversion Element of the Office of Fuels Development of the U.S. Department of Energy.

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APPENDIX A
ASPEN Plus DFMS (Data File Management System) Input File

```
TITLE 'BIOFUELS DATABASE'
;
;  Source Codes for Data
;  9 - Literature Data
;  8 - Regressed to Literature Data
;  7 - Calculated Directly (e.g. MW)
;  6 - Calculated from other Literature Data (e.g. delHf from delHc)
;  5 - Estimated using PREDICT (C)
;  4 - Estimated, but not from PREDICT (C)
;  3 - Used Literature Data for a Similar Compound on Mass Basis
;  2 - Used Literature Data for a Similar Compound on Molar Basis
;  1 - Copied from a "Similar" Compound
;  0 - Unknown Origin
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;
FILE     INHSPCD  INHSPCD  NEW
WRFILE   INHSPCD
NEW-COMP  GLUCOSE   C6H12O6         /
          XYLOSE    C5H10O5         /
          CELLULOS  C6H10O5         /
          XYLAN     C5H8O4          /
          LIGNIN    CXHXOX          /
          ZYMO      CHXOXNX         /
          BIOMASS   CHXNXOXSX-1     /
          CELLULAS  CHXNXOXSX-2     /
          SOLSLDS   CHXOXSX         /
          SOLUNKN   CXHOX           /
          GYPSUM    CASO4-2H2O
NEW-PROP                  MW     1  /       TC     1  /       PC     1  /
                          VC     1  /       TB     1  /    OMEGA     1  /
                      DHFORM     1  /   DGFORM     1  /   DGSFRM     1  /
                      DHSFRM     1  /   PLXANT     9  /   DHVLWT     5  /
                      RKTZRA     1  /   CPIG      11  /   CPSPO1     8  /
                      VSPOLY     7  ;/   CPLDIP    7  /    COMPHL    1
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Glucose
;
PROP-DATA
   PROP-LIST              MW     7  /       TC     5  /       PC     5  /
                          VC     5  /       TB     5  /    OMEGA     5  /
                      DHFORM     6  /   DGFORM     9  /   RKTZRA     8

      PVAL  GLUCOSE     180.16      /    1011.1      /   0.62000E+07  /
                     0.41650        /    825.40      /    2.5674      /
                    -1.256903E+9    /  -0.90933E+09  /   0.35852

;
   PROP-LIST              CPIG    6
      PVAL  GLUCOSE   2.07E5             0.00000           0.00000
                      0.00000            0.0.000           0.00000
                      250                1000              0.00000
                      0.00000            0.00000
;
   PROP-LIST              PLXANT   5
```

```
      PVAL   GLUCOSE      1182.2            -84682.           0.00000
                         0.15640           -175.85          -0.23777E-04
                          2.0000            573.15            993.15
;
   PROP-LIST               DHVLWT  0
      PVAL   GLUCOSE     5.02E+05           298               0.38
                         0.00000            200
;
;  PROP-LIST               CPLDIP  9
;     PVAL   GLUCOSE     2.07431E5         0.00000            0.00000
;                        0.0000            0.00000            250
;                        1000
; COMPHL required to envoke CPLDIP
;  PROP-LIST               COMPHL 0
;     PVAL GLUCOSE          1
;
;  End of Glucose Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Xylose
;
   PROP-LIST                 MW     7  /        TC     5  /        PC     5  /
                             VC     5  /        TB     5  /     OMEGA     5  /
                           DHFORM   6  /      RKTZRA 3
;
      PVAL   XYLOSE       150.132      /     890.42       /    0.65777E+07   /
                         0.34250       /     715.01       /     2.3042       /
                       -1.040002E+09 /      0.29936
;
   PROP-LIST               PLXANT  5
      PVAL   XYLOSE       481.33            -46623.           0.00000
                         0.21007E-01       -64.331            0.62243E-05
                          2.0000            573.15            873.15
;
   PROP-LIST               DHVLWT  0
      PVAL   XYLOSE      4.1868E6           298               0.38
                         0.00000            200
;
   PROP-LIST               CPIG    3
      PVAL   XYLOSE      1.7E5             0.00000            0.00000
                         0.00000           0.00000            0.00000
                         250               1000               0.00000
                         0.00000           0.00000
;
;  PROP-LIST               CPLDIP  3
;     PVAL   XYLOSE      1.72857E5         0.00000            0.00000
;                        0.0000            0.00000            250
;                        1000
; COMPHL required to envoke CPLDIP
;  PROP-LIST               COMPHL 0
;     PVAL   XYLOSE         1
;
; End of Xylose Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Cellulose
;  (Considered a Solid)
;
```

```
   PROP-LIST           MW  7       /   DHSFRM  6
      PVAL  CELLULOS  162.1436     /   -9.76362E8
;
   PROP-LIST  CPSPO1  9
      PVAL  CELLULOS  -0.11704E5         .67207E3        0.00000
                       0.0000           0.00000         0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  CELLULOS   0.10600          0.00000         0.00000
                       0.00000          0.00000          298.15
                       1000
;
; End of Cellulose Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Xylan
;  (Considered a Solid)
;
   PROP-LIST           MW  7      /    DHSFRM  2
      PVAL  XYLAN     132.117     /   -7.62416E8
;
   PROP-LIST  CPSPO1  3
      PVAL  XYLAN     -0.95363E4         .54762E3        0.00000
                       0.0000           0.00000         0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  XYLAN      0.08640          0.00000         0.00000
                       0.00000          0.00000          298.15
                       1000
;
;  End of Xylan
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Lignin
;  (Considered a Solid)
;  Formula of Lignin C7.3H13.9O1.3
;
   PROP-LIST         MW  7      /    DHSFRM  6
      PVAL  LIGNIN  122.493     /   -1.592659E9
;
   PROP-LIST  CPSPO1  9
      PVAL  LIGNIN     3.14317E4        3.94427E2       0.00000
                       0.0000           0.00000         0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  LIGNIN     0.0817           0.00000         0.00000
                       0.00000          0.00000          298.15
                       1000
;
; End of Lignin Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Cellulase (Enzyme)
;  (Considered a Solid)
;  Formula of Cellulase CH1.57N0.29O0.31S0.007
```

```
;
   PROP-LIST           MW  7   /    DHSFRM  6
      PVAL  CELLULAS  22.8398  /   -7.4944E7
;
   PROP-LIST  CPSPO1  4
      PVAL  CELLULAS   3.5533E4         0.00000          0.00000
                       0.0000           0.00000          0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  CELLULAS   0.0152           0.00000          0.00000
                       0.00000          0.00000           298.15
                       1000
;
; End of Cellulase Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Biomass - Cell Mass
;  (Considered a Solid)
;  Formula of Biomass C H1.64 N0.23 O0.39 S0.0035
;
   PROP-LIST            MW  7   /     DHSFRM  6
      PVAL  BIOMASS    23.238   /    -9.71338E7
;
   PROP-LIST  CPSPO1  4
      PVAL  BIOMASS    3.5910E4         0.00000          0.00000
                       0.0000           0.00000          0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  BIOMASS    0.01549          0.00000          0.00000
                       0.00000          0.00000           298.15
                       1000
;
; End of Biomass Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Zymo - Enzyme
;  (Considered a Solid)
;  Formula of Zymo C H1.8 O0.5 N0.2
;
   PROP-LIST            MW  7    /     DHSFRM  4
      PVAL  ZYMO       24.6264   /    -1.305E8
;
   PROP-LIST  CPSPO1  4
      PVAL  ZYMO       3.8409E4         0.00000          0.00000
                       0.0000           0.00000          0.00000
                       298.15            1000
;
   PROP-LIST  VSPOLY  3
      PVAL  ZYMO       0.0164           0.00000          0.00000
                       0.00000          0.00000           298.15
                       1000
; End of Zymo Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  SOLSLDS
;  (Considered a Mixed Component - Dissolved Solid)
```

```
;     Actual Formula: C H1.48 O.19 S.0013
;
   PROP-LIST                   MW     7  /        TC     1  /        PC     1  /
                               VC     1  /        TB     1  /     OMEGA   1  /
                           DHFORM     4  /     RKTZRA    0
;
      PVAL  SOLSLDS       16.5844      /    1011.1       /    0.62000E+07  /
                         0.41650       /    825.40       /     2.5674      /
                        -4.754E7       /    0.09908
;
   PROP-LIST                 CPIG    1
      PVAL  SOLSLDS      1.69E4            0.00000            0.00000
                         0.00000           0.00000            0.00000
                         250               1000               0.00000
                         0.00000           0.00000
;
   PROP-LIST                 PLXANT  1
      PVAL  SOLSLDS       1182.2           -84682.            0.00000
                         0.15640           -175.85           -0.23777E-04
                          2.0000            573.15             993.15
;
   PROP-LIST                 DHVLWT  0
      PVAL  SOLSLDS      4.1868E6           298               0.38
                         0.00000            200
;
;  PROP-LIST                 CPLDIP  1
;     PVAL  SOLSLDS      1.90948E4         0.00000            0.00000
;                        0.0000            0.00000            250
;                        1000
; COMPHL required to envoke CPLDIP
;  PROP-LIST                 COMPHL 0
;     PVAL  SOLSLDS          1
;  End of SOLSLDS Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  SOLUNKN (formerly Unknown)
;  (Considered a Mixed Component - Dissolved Solid)
;     Actual Formula: C H0.50 0.5
;
   PROP-LIST                   MW     7  /        TC     1  /        PC     1  /
                               VC     1  /        TB     1  /     OMEGA   1  /
                           DHFORM     4  /     RKTZRA    0
;
      PVAL  SOLUNKN       15.0134      /    890.42       /    0.65777E+07  /
                         0.34250       /    715.01       /     2.3042      /
                        -1.19E8        /   0.09404
;
   PROP-LIST                 CPIG    1
      PVAL  SOLUNKN      1.515E4           0.00000            0.00000
                         0.00000           0.00000            0.00000
                         250               1000               0.00000
                         0.00000           0.00000
;
   PROP-LIST                 PLXANT  1
      PVAL  SOLUNKN       1182.2           -84682.            0.00000
                         0.15640           -175.85           -0.23777E-04
                          2.0000            573.15             993.15
;
```

```
   PROP-LIST              DHVLWT  0
      PVAL  SOLUNKN     4.1868E6          298               0.38
                        0.00000           200
;
;  PROP-LIST              CPLDIP  1
;     PVAL  SOLUNKN     1.72860E4        0.00000           0.00000
;                       0.0000           0.00000           250
;                       1000
; COMPHL required to envoke CPLDIP
;  PROP-LIST              COMPHL 0
;     PVAL  SOLUNKN        1
;
;  End of SOLUNKN Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Gypsum
;   Solid
;  Formula of Gypsum CaSO4-2H2O
;
   PROP-LIST            MW  7    /      DHSFRM  9   /  DGSFRM  9
      PVAL  GYPSUM     172.168   /    -2.022628E9  / -1.797197E9
;
   PROP-LIST  CPSPO1  2
      PVAL  GYPSUM    7.2182E4          9.73430E1          0.00000
                       0.0000          -1.3733E8           0.00000
                       298              1400
;
   PROP-LIST  VSPOLY  9
      PVAL  GYPSUM     0.07469          0.00000            0.00000
                       0.00000          0.00000             298.15
                       1000
;
; End of Gypsum Data
;
PRINT-DIR  INHSPCD ALL
PRINT-DATA INHSPCD ALL
END-INPUT
```

APPENDIX B
ASPEN Plus PROP-DATA Input File

```
;PROP-REPLACE NRTL NRTL
;    PROP DHL DHL09
;
COMPONENTS
NEW-COMP  GLUCOSE   /
          XYLOSE    /
          CELLULOS  /
          XYLAN     /
          LIGNIN    /
          ZYMO      /
          BIOMASS   /
          CELLULAS  /
          SOLSLDS   /
          SOLUNKN
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Glucose
;
PROP-DATA
   PROP-LIST               MW        /       TC        /      PC        /
                           VC        /       TB        /      OMEGA     /
                         DHFORM      /     DGFORM      /     RKTZRA

      PVAL  GLUCOSE       180.16     /     1011.1      /   0.62000E+07 /
                         0.41650     /     825.40      /    2.5674     /
                       -1.256903E+9 /  -0.90933E+09 /   0.35852

;
   PROP-LIST              CPIG
      PVAL  GLUCOSE      2.07E5              0.00000           0.00000      &
                         0.00000             0.0.000           0.00000      &
                         250                 1000              0.00000      &
                         0.00000             0.00000
;
   PROP-LIST              PLXANT
      PVAL  GLUCOSE      1182.2             -84682.            0.00000      &
                         0.15640            -175.85          -0.23777E-04   &
                         2.0000              573.15            993.15
;
   PROP-LIST              DHVLWT
      PVAL  GLUCOSE      5.02E+05            298               0.38         &
                         0.00000             200
;
;   PROP-LIST              CPLDIP
;      PVAL  GLUCOSE      2.07431E5           0.00000           0.00000      &
;                         0.0000              0.00000           250          &
;                         1000
;  PROP-LIST               COMPHL
;     PVAL GLUCOSE           1
;
;  End of Glucose Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Xylose
;
```

```
   PROP-LIST              MW      /       TC      /       PC      /
                          VC      /       TB      /      OMEGA    /
                       DHFORM     /      RKTZRA
;
      PVAL  XYLOSE      150.132    /    890.42     /   0.65777E+07 /
                        0.34250    /    715.01     /    2.3042     /
                     -1.040002E+09 /   0.29936
;
   PROP-LIST             PLXANT
      PVAL  XYLOSE      481.33          -46623.          0.00000      &
                       0.21007E-01      -64.331          0.62243E-05  &
                        2.0000           573.15           873.15
;
   PROP-LIST             DHVLWT
      PVAL  XYLOSE     4.1868E6           298            0.38         &
                       0.00000            200
;
   PROP-LIST               CPIG
      PVAL  XYLOSE      1.7E5           0.00000          0.00000      &
                        0.00000         0.00000          0.00000      &
                        250             1000             0.00000      &
                        0.00000         0.00000
;
;   PROP-LIST             CPLDIP
;      PVAL  XYLOSE      1.72857E5        0.00000          0.00000      &
;                        0.0000           0.00000          250          &
;                        1000
;
;  PROP-LIST              COMPHL
;     PVAL  XYLOSE          1
;
; End of Xylose Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Cellulose
;  (Considered a Solid)
;
   PROP-LIST           MW          /   DHSFRM
      PVAL  CELLULOS  162.1436     /   -9.76362E8
;
   PROP-LIST  CPSPO1
      PVAL  CELLULOS  -0.11704E5        .67207E3        0.00000      &
                       0.0000          0.00000          0.00000      &
                       298.15           1000
;
   PROP-LIST  VSPOLY
      PVAL  CELLULOS   0.10600          0.00000          0.00000      &
                       0.00000          0.00000           298.15      &
                       1000
;
; End of Cellulose Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Xylan
;  (Considered a Solid)
;
   PROP-LIST           MW          /    DHSFRM
      PVAL  XYLAN     132.117      /   -7.62416E8
```

```
;
   PROP-LIST  CPSPO1
      PVAL  XYLAN     -0.95363E4          .54762E3        0.00000      &
                       0.0000            0.00000         0.00000      &
                       298.15             1000
;
   PROP-LIST  VSPOLY
      PVAL  XYLAN      0.08640           0.00000         0.00000      &
                       0.00000           0.00000          298.15      &
                       1000
;
;  End of Xylan
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Lignin
;  (Considered a Solid)
;  Formula of Lignin C7.3H13.9O1.3
;
   PROP-LIST         MW          /    DHSFRM
      PVAL  LIGNIN  122.493      /   -1.592659E9
;
   PROP-LIST  CPSPO1
      PVAL  LIGNIN     3.14317E4         3.94427E2        0.00000      &
                       0.0000            0.00000         0.00000      &
                       298.15             1000
;
   PROP-LIST  VSPOLY
      PVAL  LIGNIN     0.0817            0.00000         0.00000      &
                       0.00000           0.00000          298.15      &
                       1000
;
; End of Lignin Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\
;  Cellulase (Enzyme)
;  (Considered a Solid)
;  Formula of Cellulase CH1.57N0.29O0.31S0.007
;
   PROP-LIST           MW       /    DHSFRM
      PVAL  CELLULAS  22.8398   /   -7.4944E7
;
   PROP-LIST  CPSPO1
      PVAL  CELLULAS   3.5533E4          0.00000         0.00000      &
                       0.0000            0.00000         0.00000      &
                       298.15             1000
;
   PROP-LIST  VSPOLY
      PVAL  CELLULAS   0.0152            0.00000         0.00000      &
                       0.00000           0.00000          298.15      &
                       1000
;
; End of Cellulase Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Biomass - Cell Mass
;  (Considered a Solid)
;  Formula of Biomass C H1.64 N0.23 O0.39 S0.0035
;
```

```
   PROP-LIST              MW        /      DHSFRM
      PVAL  BIOMASS     23.238     /    -9.71338E7
;
   PROP-LIST  CPSPO1
      PVAL  BIOMASS     3.5910E4          0.00000           0.00000      &
                        0.0000            0.00000           0.00000      &
                        298.15             1000
;
   PROP-LIST  VSPOLY
      PVAL  BIOMASS     0.01549           0.00000           0.00000      &
                        0.00000           0.00000            298.15      &
                        1000
;
; End of Biomass Data
;
;\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  Zymo - Enzyme
;  (Considered a Solid)
;  Formula of Zymo C H1.8 O0.5 N0.2
;
   PROP-LIST              MW         /     DHSFRM
      PVAL  ZYMO        24.6264     /    -1.305E8
;
   PROP-LIST  CPSPO1
      PVAL  ZYMO        3.8409E4          0.00000           0.00000      &
                        0.0000            0.00000           0.00000      &
                        298.15             1000
;
   PROP-LIST  VSPOLY
      PVAL  ZYMO        0.0164            0.00000           0.00000      &
                        0.00000           0.00000            298.15      &
                        1000
;
; End of Zymo Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  SOLSLDS
;  (Considered a Mixed Component - Dissolved Solid)
;     Actual Formula: C H1.48 O.19 S.0013
;
   PROP-LIST                 MW        /       TC        /       PC        /
                             VC        /       TB        /      OMEGA      /
                           DHFORM      /     RKTZRA
;
      PVAL  SOLSLDS       16.5844     /     1011.1      /   0.62000E+07  /
                          0.41650     /     825.40      /    2.5674      /
                         -4.754E7     /     0.09908
;
   PROP-LIST                CPIG
      PVAL  SOLSLDS     1.69E4            0.00000           0.00000      &
                        0.00000           0.00000           0.00000      &
                        250               1000              0.00000      &
                        0.00000           0.00000
;
   PROP-LIST                PLXANT
      PVAL  SOLSLDS      1182.2           -84682.           0.00000      &
                         0.15640          -175.85         -0.23777E-04   &
                         2.0000            573.15           993.15
```

```
;
  PROP-LIST                DHVLWT
     PVAL  SOLSLDS       4.1868E6          298              0.38         &
                         0.00000           200
;
;  PROP-LIST                CPLDIP
;     PVAL  SOLSLDS      1.90948E4         0.00000          0.00000      &
;                        0.0000            0.00000          250          &
;                        1000
;
;  PROP-LIST                COMPHL
;     PVAL  SOLSLDS         1
;
;  End of SOLSLDS Data
;
;/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/\/
;  SOLUNKN (formerly Unknown)
;  (Considered a Mixed Component - Dissolved Solid)
;     Actual Formula: C H0.50 0.5
;
   PROP-LIST                 MW       /      TC       /       PC        /
                             VC       /      TB       /      OMEGA      /
                           DHFORM     /    RKTZRA
;
      PVAL  SOLUNKN      15.0134      /    890.42     /   0.65777E+07   /
                         0.34250      /    715.01     /    2.3042       /
                        -1.19E8       /   0.09404
;
   PROP-LIST               CPIG
      PVAL  SOLUNKN      1.515E4           0.00000          0.00000      &
                         0.00000           0.00000          0.00000      &
                         250               1000             0.00000      &
                         0.00000           0.00000
;
   PROP-LIST               PLXANT
      PVAL  SOLUNKN      1182.2           -84682.           0.00000      &
                         0.15640          -175.85          -0.23777E-04  &
                         2.0000            573.15           993.15
;
   PROP-LIST               DHVLWT
      PVAL  SOLUNKN      4.1868E6          298              0.38         &
                         0.00000           200
;
;  PROP-LIST                CPLDIP
;     PVAL  SOLUNKN      1.72860E4         0.00000          0.00000      &
;                        0.0000            0.00000          250          &
;                        1000
;
;  PROP-LIST               COMPHL
;     PVAL  SOLUNKN         1
;
;  End of SOLUNKN Data
;
```

APPENDIX C																	
Compound	Primary Phase	Database Alias	Quality of Properties in INHSPCD Databank for ASPEN Plus														
			Single Point Values								Temperature Correlations						
			MW	TC	PC	VC	OMEGA	DHFORM	DGFORM	DHSFRM	RKTZRA	PLXANT	DHVLWT	CPIG	CPLDIP	CPSPO1*	VSPOLY*
Glucose	VL	C6H12O6	7	5	5	5	5	6	9		8	5	0	6	9		
Xylose	VL	C5H10O5	7	5	5	5	5	6			3	5	0	3	3		
Cellulose	S	C6H10O5	7							6						9	3
Xylan	S	C5H8O4	7							2						3	3
Lignin	S	CXHXOX	7							6						9	3
Zymo	S	CHXOXNX	7							4						4	3
Cellulas	S	CHXNXOXSX-2	7							6						4	3
Biomass	S	CHXNXOXSX-1	7							6						4	3
Solunkn	VL	CXHOX	7	1	1	1	1	4			0	1	0	1	3		
SolSlds	VL	CHXOXSX	7	1	1	1	1	4			0	1	0	1	3		
Gypsum	S	CASO4-2H2O	7							9						2	9

*Solid Properties

Source Codes for Data

9 - Literature Data

8 - Regressed to Literature Data

7 - Calculated Directly (e.g. MW)

6 - Calculated from other Literature Data (e.g. delHf from delHc)

5 - Estimated using PREDICT (C)

4 - Estimated, but not from PREDICT (C)

3 - Used Literature Data for a Similar Compound on Mass Basis

2 - Used Literature Data for a Similar Compound on Molar Basis

1 - Copied from a "Similar" Compound

0 - Unknown Origin

Appendix D
Values in ASPEN Plus INHSPCD (NREL Biofuels) Databank

Property	Aspen Property	Units	Glucose	Xylose	Cellulose	Xylan	Lignin	Cellulase	Zymo	Biomass	Solslds	Solunkn	Gypsum
Molecular Weight	MW		180.16	150.132	162.1436	132.117	122.493	22.8398	24.6264	23.238	16.5844	15.0134	172.168
Critical Temperature	TC	K	1011.1	890.42							1011.1	890.42	
Critical Pressure	PC	Pascal	6,200,000	6,577,700							6,200,000	6,577,700	
Critical Volume	VC	cum/Kmole	0.4165	0.3425							0.4165	0.3425	
Acentric Factor	OMEGA		2.5674	2.3042							2.5674	2.3042	
I.G. Heat of Formation	DHFORM	J/Kmole	-1,256,903,000	-1,040,020,000							-47,540,000	-119,000,000	
I.G. Free Energy of Form.	DGFORM	J/Kmole	-909,330,000										
Solid Heat of Formation	DHSFRM	J/Kmole			-976,362,000	-762,416,000	-1,592,659,000	-74,944,000	-130,500,000	-97,133,800			-2,022,628,000
Solid Free Energy of Form.	DGSFRM	J/Kmole											-1,797,197,000
Vapor Pressure	PLXANT/1	Pascal	1182.2	481.33							1182.2	1182.2	
	PLXANT/2		-84682	-46623							-84682	-84682	
	PLXANT/3		0	0							0	0	
	PLXANT/4		0.1564	2.10E-02							0.1564	0.1564	
	PLXANT/5		-175.85	64.331							-175.85	-175.85	
	PLXANT/6		-2.37770E-05	6.22430E-06							-2.37770E-05	-2.37770E-05	
	PLXANT/7		2	2							2	2	
	PLXANT/8		573.15	573.15							573.15	573.15	
	PLXANT/9		993.15	873.15							993.15	993.15	
Heat of Vaporization	DHVLWT/1	J/Kmole	502,000	4,186,800							4,186,800	4,186,800	
	DHVLWT/2		298	298							298	298	
	DHVLWT/3		0.38	0.38							0.38	0.38	
	DHVLWT/4		0	0							0	0	
	DHVLWT/5		200	200							200	200	
Liquid Molar Volume	RKTZRA	cum/Kmole	0.35852	0.29936							0.09908	0.09404	
Solid Molar Volume	VSPOLY/1	cum/Kmole			0.106	0.0864	0.0817	0.0152	0.0164	0.01549			0.07469
	VSPOLY/2				0	0	0	0	0	0			0
	VSPOLY/3				0	0	0	0	0	0			0
	VSPOLY/4				0	0	0	0	0	0			0
	VSPOLY/5				0	0	0	0	0	0			0
	VSPOLY/6				298.15	298.15	298.15	298.15	298.15	298.15			298.15
	VSPOLY/7				1000	1000	1000	1000	1000	1000			1000
I.G. Heat Capacity	CPIG/1	J/Kmole K	207,000	170,000							16,900	15,150	
	CPIG/2		0	0							0	0	
	CPIG/3		0	0							0	0	
	CPIG/4		0	0							0	0	
	CPIG/5		0	0							0	0	
	CPIG/6		0	0							0	0	
	CPIG/7		250	250							250	250	
	CPIG/8		1000	1000							1000	1000	
	CPIG/9		0	0							0	0	
	CPIG/10		0	0							0	0	
	CPIG/11		0	0							0	0	
Solid Heat Capacity	CPSPO1/1	J/Kmole K			-11704	-9529.9	31431.7	35533	38409	35910			72,182
	CPSPO1/2				672.07	547.25	394.427	0	0	0			97.343
	CPSPO1/3				0	0	0	0	0	0			0
	CPSPO1/4				0	0	0	0	0	0			0
	CPSPO1/5				0	0	0	0	0	0			-137,330,000
	CPSPO1/6				0	0	0	0	0	0			0.00E+00
	CPSPO1/7				298.15	298.15	298.15	298.15	298.15	298.15			298
	CPSPO1/8				1000	1000	1000	1000	1000	1000			1400
Liquid Heat Capacity	CPLDIP/1	J/Kmole K	207431	172857							19094	17286	
	CPLDIP/2		0	0							0	0	
	CPLDIP/3		0	0							0	0	
	CPLDIP/4		0	0							0	0	
	CPLDIP/5		0	0							0	0	
	CPLDIP/6		250	250							250	250	
	CPLDIP/7		1000	1000							1000	1000	

APPENDIX E
Data Values in ASPEN Plus NREL Biofuels INHSPCD Databank

Temperature Correlations Used in ASPEN Plus

Vapor Pressure - PLXANT

$$\ln p_i^{*,l} = C_{1i} + \frac{C_{2i}}{T + C_{3i}} + C_{4i}T + C_{5i}\ln T + C_{6i}T^{C_{7i}} \quad \text{for} \quad C_{8i} \le T \le C_{9i}$$

Where,

PLXANT/1....9 correspond to C_{1i}....$_{9i}$

Watson Heat of Vaporization - DHVLWT

$$\Delta_{vap}H_i^*(T) = \Delta_{vap}H_i^*(T_1)\left(\frac{1 - T/T_{ci}}{1 - T_1/T_{ci}}\right)^{a_i + b_i(1 - T/T_{ci})} \quad \text{for} \quad T > T_{min}$$

Where,

$\Delta_{vap}H_i^*(T_1)$ = Heat of Vaporization at temperature T_1

Parameter	Symbol
TC	T_{ci}
DHVLWT/1	$\Delta_{vap}H_i^*(T_1)$
DHVLWT/2	T_1
DHVLWT/3	a_i
DHVLWT/4	b_i
DHVLWT/5	T_{min}

Rackett Liquid Molar Volume - RKTZRA

$$V_m^l = \frac{RT_c(Z_m^{RA})^{[1+(1-T_r)^{2/7}]}}{p_c}$$

Where,

$$Tc = \sum_i \sum_j x_i x_j V_{ci} V_{cj} (T_{ci} T_{cj})^{1/2} (1 - k_{ij}) / V_{cm}^2$$

$$\frac{T_c}{p_c} = \sum_i x_i \frac{T_{ci}}{p_{ci}}$$

$$Z_m^{RA} = \sum_i x_i Z_i^{*,RA}$$

$$V_{cm} = \sum_i x_i V_{ci}$$

$$T_r = \frac{T}{T_c}$$

Rackett Liquid Molar Volume - RKTZRA - Continued

Parameter	Symbol
TC	T_{ci}
PC	p_{ci}
VC	V_{ci}
RKTZRA	Z_i^{RA}
RKTKIJ	k_{ij}

Solids Volume Polynomial - VSPOLY

$$V_i^{*,s}(T) = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 \quad \text{for} \quad C_{6i} \le T \le C_{7i}$$

Where,

VSPOLY/1....7 correspond to $C_{1i\cdots 7i}$

Ideal Gas Heat Capacity - CPIG

$$C_p^{*,ig}(T) = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 + C_{6i}T^5 \quad \text{for} \quad C_{7i} \le T \le C_{8i}$$
$$C_p^{*,ig}(T) = C_{9i} + C_{10i}T \quad \text{for} \quad T < C_{7i}$$

Where,

CPIG/1....11 correspond to $C_{1i\cdots 11i}$

Solids Heat Capacity

$$C_{p,i}^{*,s}(T) = C_{1i} + C_{2i}T + C_{3i}T^2 + \frac{C_{4i}}{T} + \frac{C_{5i}}{T^2} + \frac{C_{6i}}{\sqrt{T}} \quad \text{for} \quad C_{7i} \le T \le C_{8i}$$

Where,

CPSP01/1....8 correspond to $C_{1i\cdots 8i}$

DIPPR Liquid Heat Capacity - CPLDIP

$$C_{p,i}^{*,l}(T) = C_{1i} + C_{2i}T + C_{3i}T^2 + C_{4i}T^3 + C_{5i}T^4 \quad \text{for} \quad C_{6i} \le T \le C_{7i}$$

Where,

CPLDIP/1....7 correspond to $C_{1i\cdots 7i}$

APPENDIX F
ASPEN Plus Physical Property Route Modifications to Enable the DIPPR Liquid Heat Capacity Correlation

The standard physical property calculation route in ASPEN PLUS does not use a correlation for liquid heat capacity; rather, it uses correlations for the ideal gas heat capacity and the heat of vaporization. For some compounds studied here, which exist in the liquid phase, a liquid heat capacity rather than a heat of vaporization or gas heat capacity was available. To take advantage of these data, the DIPPR correlation for liquid heat capacity (available in ASPEN PLUS) was used. To enable this model, a modification to the physical property route was necessary. This modification is:

```
PROP-REPLACE NRTL NRTL
  PROP DHL DHL09
```

These imput language statements (also available in Model Manager) modify the basic physical property option set, NRTL, to use the DIPPR liquid heat capacity route, DHL09, for the calculation of liquid enthalpy, DHL09.

With this modification, the DIPPR liquid heat capacity model will be used only if data are present. If no data are present for this model (CPLDIP), the calculations will revert to the standard methods of using the IG heat capacity and heat of vaporization.

This method has a bug in it that Aspen Technology is not willing to fix at this time. Therefore, even though this was a good method for calculating the necessary liquid heat capacity, it was not available as of this writing.

REPORT DOCUMENTATION PAGE

Form Approved
OMB NO. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	April 1996	NREL Report

4. TITLE AND SUBTITLE

Development of a Biofuels Physical Property Database for ASPEN+ Simulators

5. FUNDING NUMBERS

BF521004

6. AUTHOR(S)

R.J. Wooley, V. Putsche

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401

8. PERFORMING ORGANIZATION REPORT NUMBER

DE96007902

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

National Renewable Energy Laboratory
1617 Cole Boulevard
Golden, CO 80401-3393

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

NREL/TP-425-20685

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

National Technical Information Service
U.S. Department of Commerce
5285 Port Royal Road
Springfield, VA 22161

12b. DISTRIBUTION CODE

UC-1503

13. ABSTRACT *(Maximum 200 words)*

Physical property data for many key components used to simulate ethanol from biomass are not available in the standard ASPEN PLUS property databases. Therefore, we must evaluate the literature, estimate properties, and determine a set of consistent physical properties for all components of interest. The components must then be entered into a in-house NREL ASPEN PLUS database so they can be called on without being retyped into each specific simulation.

14. SUBJECT TERMS

simulator, physical properties, vapor pressure, heat of vaporization, liquid density

15. NUMBER OF PAGES

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT

NSN 7540-01-280-5500

Standard Form 298 (Rev. 2-89)
Prescribed by ANSI Std. Z39-18
298-102