Use of spectroscopy analysis and computational chemistry for rice husk and gluten husk applications

Norma A. Rangel-Vazquez
Virginia Hernandez-Montoya
Adrian Bonilla-Petriciolet

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Use of Spectroscopy Analysis and Computational Chemistry for Rice Husk and Gluten Husk Applications

Norma-Aurea Rangel-Vazquez*, Virginia Hernandez-Montoya and Adrian Bonilla-Petriciolet

Division of Graduate Studies and Research, Aguascalientes, México

Abstract
Computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. It uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids. The lignocellulosic materials are mainly made up of a complex network of three polymers: cellulose, hemicellulose, and lignin. Due to their hydrophilicity, biodegradability, biocompatibility and low toxicity, hemicelluloses have been studied by numerous research groups with respect to their use as composites in biomedical applications.

In this research, rice husk and gluten husk were analyzed. Rice husk (RH) is a fibrous material, composed mainly of cellulose, lignin and inorganic and organic compounds. Rice husk ash (RHA) is a light material, which is bulky and porous; it amounts to about 20% of the burnt husk. Gluten is the composite of a gliadin and a glutenin, which is conjoined with starch in the endosperm of various grass-related grains. The prolamin and glutelin from wheat (gliadin, which is alcohol-soluble, and glutenin, which is only soluble in dilute acids or alkalis) constitute about 80% of the protein contained in wheat fruit.

The analysis techniques used were: FTIR to study this effect and the optional use of theoretical calculationsto justify the obtained results by means of computational chemistry tools. Using QSAR properties, we can obtain an estimate of the activity of a chemical from its molecular structure only. The QSARs have been successfully applied to predict soil sorption coefficients of non-polar and nonionizable organic compounds, including many pesticides. Sorption of organic chemicals in soils or sediments is usually described by sorption coefficients. The molecular electrostatic potential (MESP) was calculated using the AMBER/AM1 method. These methods give information about the proper region by which compounds have intermolecular interactions between their units.

Keywords: Lignocellulosic materials, absorption process, computational chemistry, geometry optimization, QSAR, FTIR, potential electrostatic

*Corresponding author: normarangelvazquez201301@gmail.com
8.1 Introduction

8.1.1 Computational Chemistry

Computational chemistry is a branch of chemistry that uses principles of computer science to assist in solving chemical problems. It uses the results of theoretical chemistry, incorporated into efficient computer programs, to calculate the structures and properties of molecules and solids. Its necessity arises from the well-known fact that apart from relatively recent results concerning the hydrogen molecular ion (see references therein for more details), the quantum many-body problem cannot be solved analytically, much less in closed form. While its results normally complement the information obtained by chemical experiments, it can in some cases predict hitherto unobserved chemical phenomena. It is widely used in the design of new drugs and materials. Examples of such properties are structure (i.e., the expected positions of the constituent atoms), absolute and relative (interaction) energies, electronic charge distributions, dipoles and higher multipole moments, vibrational frequencies, reactivity or other spectroscopic quantities, and cross-sections for collision with other particles.

In all cases the computer time and other resources (such as memory and disk space) increase rapidly with the size of the system being studied. That system can be a single molecule, a group of molecules, or a solid. Computational chemistry methods range from highly accurate to very approximate; highly accurate methods are typically feasible only for small systems [1].

A single molecular formula can represent a number of molecular isomers. Each isomer is a local minimum on the energy surface (called the potential energy surface) created from the total energy (i.e., the electronic energy, plus the repulsion energy between the nuclei) as a function of the coordinates of all the nuclei. A stationary point is geometry such that the derivative of the energy with respect to all displacements of the nuclei is zero. A local (energy) minimum is a stationary point where all such displacements lead to an increase in energy. The local minimum that is lowest is called the global minimum and corresponds to the most stable isomer. If there is one particular coordinate change that leads to a decrease in the total energy in both directions, the stationary point is a transition structure and the coordinate is the reaction coordinate. This process of determining stationary points is called geometry optimization.

The determination of molecular structure by geometry optimization became routine only after efficient methods for calculating the first derivatives of the energy with respect to all atomic coordinates became available. Evaluation of the related second derivatives allows the prediction of vibrational frequencies if harmonic motion is estimated. More importantly, it allows for the characterization of stationary points. The frequencies are related to the Eigenvalues of the Hessian matrix, which contains second derivatives. If the Eigenvalues are all positive, then the frequencies are all real and the stationary point is a local minimum. If one Eigenvalue is negative (i.e., an imaginary frequency), then the stationary point is a transition structure. If more than one Eigenvalue is negative, then the stationary point is a more complex one, and is usually of little interest.

When one of these is found, it is necessary to move the search away from it if the experimenter is looking solely for local minima and transition structures. The total energy is determined by approximate solutions of the time-dependent Schrödinger
equation, usually with no relativistic terms included, and by making use of the Born–
Oppenheimer approximation, which allows for the separation of electronic and nuclear
motions, thereby simplifying the Schrödinger equation. This leads to the evaluation
of the total energy as a sum of the electronic energy at fixed nuclei positions and the
repulsion energy of the nuclei. A notable exception is certain approaches called direct
quantum chemistry, which treat electrons and nuclei on a common footing. Density
functional methods and semi-empirical methods are variants on the major theme.
For very large systems, the relative total energies can be compared using molecular
mechanics [2,3].

8.1.1.1 Molecular Mechanics Methods

Molecular mechanics uses classical mechanics to model molecular systems. The
potential energy of all systems in molecular mechanics is calculated using force fields.
Molecular mechanics can be used to study small molecules as well as large biological
systems or material assemblies with many thousands to millions of atoms. All-atomistic
molecular mechanics methods have the following properties:

- Each atom is simulated as a single particle.
- Each particle is assigned a radius (typically the van der Waals radius),
polarizability, and a constant net charge (generally derived from quantum
calculations and/or experiment).
- Bonded interactions are treated as "springs" with an equilibrium distance
equal to the experimental or calculated bond length.

Molecular mechanics potential energy functions have been used to calculate binding
constants, protein folding kinetics, protonation equilibria, active site coordinates, and
to design binding sites [4,5].

8.1.1.1.1 AMBER Method

The term "AMBER force field" generally refers to the functional form used by the family
of AMBER force fields. This form includes a number of parameters; each member of
the family of AMBER force fields provides values for these parameters and has its own
name. The functional form of the AMBER force field is (equation 8.1).

\[
V (r^N) = \sum_{\text{bonds}} k_b (r_i - r_i^0)^2 + \sum_{\text{angles}} k_a (\theta_i - \theta_i^0)^2 + \sum_{\text{angles}} \frac{1}{2} V_N [1 + \cos (nw - \gamma)] + \sum_{\text{coul}} \sum_{\text{rep}} 4\pi\varepsilon_\alpha\varepsilon_\beta \frac{q_i q_j}{r_{ij}}
\] (8.1)

The meanings of right hand side terms are:

1. First term (summing over bonds): represents the energy between
   covalently bonded atoms. This harmonic (ideal spring) force is a good
approximation near the equilibrium bond length, but becomes increasingly poor as atoms separate.

2. Second term (summing over angles): represents the energy due to the geometry of electron orbitals involved in covalent bonding.

3. Third term (summing over torsions): represents the energy for twisting a bond due to bond order (e.g., double bonds) and neighboring bonds or lone pairs of electrons. Note that a single bond may have more than one of these terms, such that the total torsional energy is expressed as a Fourier series.

4. Fourth term (double summation over i and j): represents the non-bonded energy between all atom pairs, which can be decomposed into van der Waals (first term of summation) and electrostatic (second term of summation) energies.

The form of the van der Waals energy is calculated using the equilibrium distance \( (r_{ij}) \) and well depth \( (\epsilon) \). The factor of 2 ensures that the equilibrium distance is \( r_{ij} \). The energy is sometimes reformulated in terms of \( o \), where \( r_{ij} = 2^{1/6} (o) \), as used, e.g., in the implementation of the soft core potentials. The form of the electrostatic energy used here assumes that the charges due to the protons and electrons in an atom can be represented by a single point charge (or in the case of parameter sets that employ lone pairs, a small number of point charges) [6].

8.1.1.2 Semi-Empirical Methods

Semi-empirical quantum chemistry methods are based on the Hartree–Fock formalism, but make many approximations and obtain some parameters from empirical data. They are very important in computational chemistry for treating large molecules where the full Hartree–Fock method without the approximations is too expensive. The use of empirical parameters appears to allow some inclusion of electron correlation effects into the methods. Within the framework of Hartree–Fock calculations, some pieces of information (such as two-electron integrals) are sometimes approximated or completely omitted.

In order to correct for this loss, semi-empirical methods are parametrized, that is their results are fitted by a set of parameters, normally in such a way as to produce results that best agree with experimental data, but sometimes to agree with \textit{ab initio} results. Semi-empirical methods follow what are often called empirical methods where the two-electron part of the Hamiltonian is not explicitly included.

For π-electron systems, this was the Hückel method proposed by Erich Hückel. For all valence electron systems, the extended Hückel method was proposed by Roald Hoffmann. Semi-empirical calculations are much faster than their \textit{ab initio} counterparts. Their results, however, can be very wrong if the molecule being computed is not similar enough to the molecules in the database used to parametrize the method. Semi-empirical calculations have been most successful in the description of organic chemistry, where only a few elements are used extensively and molecules are of moderate size. However, semi-empirical methods were also applied to solids and nanostructures but with different parameterization. As with empirical methods, we can distinguish if:
Restricted to π-electrons. These methods exist for the calculation of electronically excited states of polyenes, both cyclic and linear. These methods, such as the Pariser–Parr–Pople method (PPP), can provide good estimates of the π-electronic excited states, when parameterized well. Indeed, for many years, the PPP method outperformed ab initio excited state calculations [6].

8.1.1.2.1 AM1 Method

AM1 is basically a modification to and a reparameterization of the general theoretical model found in MNDO. Its major difference is the addition of Gaussian functions to the description of core repulsion function to overcome MNDO’s hydrogen bond problem. Additionally, since the computer resources were limited in 1970s, in MNDO parameterization methodology, the overlap terms, \( \beta_s \) and \( \beta_p \), and Slater orbital exponent’s \( \zeta_s \) and \( \zeta_p \) for \( s \) - and \( p \) - atomic orbitals were fixed. That means they are not parameterized separately just considered as \( \beta_s = \beta_p \), and \( \zeta_s = \zeta_p \) in MNDO. Due to the greatly increasing computer resources in 1985 comparing to 1970s, these inflexible conditions were relaxed in AM1 and then likely better parameters were obtained.

The addition of Gaussian functions significantly increased the numbers of parameters to be parameterized from 7 (in MNDO) to 13-19, but AM1 represents a very real improvement over MNDO, with no increase in the computing time needed. Dewar also concluded that the main gains of AM1 were its ability to reproduce hydrogen bonds and the promise of better estimation of activation energies for reactions. However, AM1 has some limitations. Although hypervalent molecules are improved over MNDO, they still give larger errors than the other compounds, alkyl groups are too stable, nitro compounds are too unstable, peroxide bond are too short. AM1 has been used very widely because of its performance and robustness compared to previous methods. This method has retained its popularity for modeling organic compounds and results from AM1 calculations continue to be reported in the chemical literature for many different applications.

AM1 is currently one of the most commonly used of the Dewar-type methods. It was the next semiempirical method introduced by Dewar and coworkers in 1985 following MNDO. It is simply an extension, a modification to and also a reparameterization of the MNDO method. AM1 differs from MNDO by mainly two ways. The first difference is the modification of the core repulsion function. The second one is the parameterization of the overlap terms \( \beta_s \) and \( \beta_p \), and Slater-type orbital exponents \( \zeta_s \) and \( \zeta_p \) on the same atom independently, instead of setting them equal as in MNDO. MNDO had a very strong tendency to overestimate repulsions between atoms when they are at approximately their van der Waals distance apart. To overcome this hydrogen bond problem, the net electrostatic repulsion term of MNDO, \( f(R_{AH}) \) given by equation (1.2), was modified in MNDO/H to be

\[
f(R_{AH}) = Z_A Z_B \left( S_A S_A^* S_H S_H^* \right) \left[ e^{-\alpha R_{AH}^2} \right] \tag{8.2}
\]

Where \( \alpha \) was proposed to be equal to 2.0 Å\(^2\) for all A-H pairs. On the other hand, the original core repulsion function of MNDO was modified in AM1 by adding Gaussian functions to provide a weak attractive force. The core-core repulsion energy term in AM1 is given by equation 8.3.
The Gaussian functions $F(A)$ and $F(B)$ are expressed by equation 8.4.

\[
F(A) = \sum_i K_A \text{e}^{-(R_{AB} - M_{A,i})^2} \\
F(B) = \sum_i K_B \text{e}^{-(R_{AB} - M_{B,i})^2}
\]  

(8.4)

And finally AM1 core-repulsion function becomes (equation 8.5).

\[
E_{\text{AM1}}^{\text{MNDO}} = E_{\text{MNDO}}^{\text{AB}} + \frac{Z_A Z_B}{R_{AB}} \left( \sum_i K_{A,i} \text{e}^{-(R_{AB} - M_{A,i})^2} + \sum_j K_{B,j} \text{e}^{-(R_{AB} - M_{B,j})^2} \right)
\]  

(8.5)

In this equation 8.5, $K$, $L$, and $M$ are the Gaussian parameters. The remaining parameters have the same meaning as in the previous section. $L$ parameters determine the widths of the Gaussians and were not found to be critical by Dewar. Therefore, a common value was used for many of the $L$ parameters. On the other hand, all $K$ and $M$ parameters were optimized. Each atom has up to four of the Gaussian parameters, i.e., $K_1$, $K_2$, $L_1$, $L_2$, $M_1$, $M_2$.

Carbon has four terms in its Gaussian expansion whereas hydrogen and nitrogen have three and oxygen has two terms (only $K_1$, $K_2$, $L_1$, $L_2$, $M_1$, $M_2$). Because in AM1 for carbon, hydrogen and nitrogen both attractive and repulsive Gaussians were used whereas for oxygen only repulsive ones considered, addition of Gaussian functions into the core-repulsion function significantly increased the number of parameters to be optimized and made the parameterization process more difficult.

As for original MNDO, one-center two-electron repulsion integrals $g_{ss}$, $g_{pp}$, $g_{dd}$, $g_{sp}$, $h_{sp}$ are assigned to atomic spectral values and not optimized. In contrast to MNDO, in which parameters were first optimized for carbon and hydrogen together and then other elements added one at a time, by increased computer resources and improved optimization procedure a larger reference parameterization dataset was used in the parameterization of AM1. All the parameters for H, C, N and O were optimized at once in a single parameterization procedure.

Optimization of the original AM1 elements was performed manually by Dewar using chemical knowledge and intuition. He also kept the size of the reference parameterization data at a minimum by very carefully selecting necessary data to be used as reference. Over the following years many of the main-group elements have been parameterized keeping the original AM1 parameters for H, C, N and O unchanged. Of course, a sequential parameterization scheme caused every new parameterization to depend on previous ones, which directly affects the quality of the results.

AM1 represented a very considerable improvement over MNDO without any increase in the computing time needed. AM1 has been parameterized for many of the main-group elements and is very widely used, keeping its popularity in organic compounds' modeling due to its good performance and robustness. Although many of the deficiencies in MNDO were corrected in AM1, it still has some important limitations as outlined in the historical development section [6].
8.1.2  Lignocellulosic Materials

Lignocellulosic materials comprising forestry, agricultural and agro-industrial wastes are abundant, renewable and inexpensive energy sources. Such wastes include a variety of materials such as sawdust, poplar trees, sugarcane bagasse, waste paper, brewer’s spent grains, switch grass, and straws, stems, stalks, leaves, husks, shells and peels from cereals like rice, wheat, corn, sorghum and barley, among others [7,8].

Lignocellulose wastes are accumulated every year in large quantities, causing environmental problems. However, due to their chemical composition based on sugars and other compounds of interest, they could be utilized for the production of a number of value added products, such as ethanol, food additives, organic acids, enzymes, and others. Therefore, besides the environmental problems caused by their accumulation in the nature, the non-use of these materials constitutes a loss of potentially valuable sources. The major constituents of lignocellulose are cellulose, hemicellulose, and lignin, polymers that are closely associated with each other constituting the cellular complex of the vegetal biomass. Basically, cellulose forms a skeleton which is surrounded by hemicellulose and lignin (Figure 8.1).

Cellulose is a high molecular weight linear homopolymer of repeated units of cellobiose (two anhydrous glucose rings joined via a β-1,4 glycosidic linkage). The long-chain cellulose polymers are linked together by hydrogen and van der Walls bonds, which cause the cellulose to be packed into microfibrils. By forming these hydrogen bounds, the chains tend to arrange in parallel and form a crystalline structure. Therefore, cellulose microfibrils have both highly crystalline regions (around 2/3 of the total cellulose) and less-ordered amorphous regions. More ordered or crystalline cellulose is less soluble and less degradable.

Hemicellulose is a linear and branched heterogeneous polymer typically made up of five different sugars – L-arabinose, D-galactose, D-glucose, D-mannose, and D-xylose - as well as other components such as acetic, gluconic, and ferulic acids. The backbone of the chains of hemicelluloses can be a homopolymer (generally consisting of single sugar repeat unit) or a heteropolymer (mixture of different sugars). According to the main sugar residue in the backbone, hemicellulose has different classifications, e.g., xylans, mannans, glucans, glucuronoxylans, arabinoxylans, glucomannans, galactomannans, galactoglucomannans, β-glucans, and xyloglucans. When compared to cellulose, hemicelluloses differ thus by composition of sugar units, by presence of shorter chains, by a branching of main chain molecules, and to be amorphous, which made its structure easier to hydrolyze than cellulose.
Lignin is a very complex molecule constructed of phenylpropane units linked in a large three-dimensional structure. Three phenyl propionic alcohols exist as monomers of lignin: p-coumaryl alcohol, coniferyl alcohol and sinapyl alcohol. Lignin is closely bound to cellulose and hemicellulose and its function is to provide rigidity and cohesion to the material cell wall, to confer water impermeability to xylem vessels, and to form a physic-chemical barrier against microbial attack. Due to its molecular configuration, lignins are extremely resistant to chemical and enzymatic degradation.

The amounts of carbohydrate polymers and lignin vary from one plant species to another. In addition, the ratios between various constituents in a single plant may also vary with age, stage of growth, and other conditions. However, cellulose is usually the dominant structural polysaccharide of plant cell walls (35–50%), followed by hemicellulose (20–35%) and lignin (10–25%). Average values of the main components in some lignocellulose wastes are shown in Table 8.1 [8].

### Table 8.1 Main components of lignocellulose wastes

<table>
<thead>
<tr>
<th>Lignocellulosic materials waste</th>
<th>Cellulose (Wt%)</th>
<th>Hemicellulose (Wt%)</th>
<th>Lignin (Wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Barley straw</td>
<td>33.8</td>
<td>21.9</td>
<td>13.8</td>
</tr>
<tr>
<td>Corn cobs</td>
<td>33.7</td>
<td>31.9</td>
<td>06.1</td>
</tr>
<tr>
<td>Corn stalks</td>
<td>35.0</td>
<td>16.8</td>
<td>07.0</td>
</tr>
<tr>
<td>Cotton stalks</td>
<td>58.5</td>
<td>14.4</td>
<td>21.5</td>
</tr>
<tr>
<td>Oat straw</td>
<td>39.4</td>
<td>27.1</td>
<td>17.5</td>
</tr>
<tr>
<td>Rice straw</td>
<td>36.2</td>
<td>19.0</td>
<td>09.9</td>
</tr>
<tr>
<td>Rye straw</td>
<td>37.6</td>
<td>30.5</td>
<td>19.0</td>
</tr>
<tr>
<td>Soya stalks</td>
<td>34.5</td>
<td>24.8</td>
<td>19.8</td>
</tr>
<tr>
<td>Sugarcane bagasse</td>
<td>40.0</td>
<td>27.0</td>
<td>10.0</td>
</tr>
<tr>
<td>Sunflower stalks</td>
<td>42.1</td>
<td>29.7</td>
<td>13.4</td>
</tr>
<tr>
<td>Wheat straw</td>
<td>32.9</td>
<td>24.0</td>
<td>08.9</td>
</tr>
</tbody>
</table>

### 8.1.2.1 Rice Husk

Rice husk ask (Figure 8.2) is one of the most widely available agricultural wastes in many rice producing countries around the world. In majority of rice producing countries much of the husk produced from processing of rice is either burnt or dumped as waste. Burning of rice husk ask in ambient atmosphere leaves a residue, called rice husk ash. For every 1000 kgs of paddy milled, about 220 kgs (22%) of husk is produced, and when this husk is burnt in the boilers, about 55 kgs (25%) of rice husk ask is generated.

The chemical composition of rice husk ask is similar to that of many common organic fibers and it contains of cellulose 40-50%, lignin 25-30%, ash 15-20% and moisture 8-15%. Typical analyses of rice husk ask is shown in Table 8.2. The content of each of them depends on rice variety, soil chemistry, climatic conditions, and even the geographic localization of the culture.
The exterior of rice husk ash are composed of dentate rectangular elements, which themselves are composed mostly of silica coated with a thick cuticle and surface hairs. The mid region and inner epidermis contain little silica. Jauberthie et al., confirmed that the presence of amorphous silica is concentrated at the surfaces of the rice husk and not within the husk itself [9]. The properties of rice husk ash and its main composition are presented in Table 8.3. The organic materials consist of cellulose and lignin which turn to CO$_2$ and CO when rice husk ash burns in air. The ash contains mainly silica (90%), and a small portion of metal oxides (~5%) and residual carbon obtained from open burning [10].

8.1.2.2 Wheat Gluten Husk

Wheat gluten is a protein composite found in foods processed from wheat and related grain species, including barley and rye. WG gives elasticity to dough, helping it rise and keep its shape and often gives the final product a chewy texture. WG may also
be found in some cosmetics, hair products, and other dermatological preparations [11,12]. Commercial WG has a mean composition of 72.5% protein (77.5% on dry basis), 5.7% total fat, 6.4% moisture and 0.7% ash; carbohydrates, mainly starches, are the other major component [13]. WG husk is the composite of a gliadin and a glutenin (Figure 8.3), which is conjoined with starch in the endosperm of various grass-related grains. The prolamin and glutelin from wheat (gliadin, which is alcohol-soluble, and glutenin, which is only soluble in dilute acids or alkalis) constitute about 80% of the protein contained in wheat fruit. Being insoluble in water, they can be purified by washing away the associated starch. Worldwide, gluten is a source of protein, both in foods prepared directly from sources containing it, and as an additive to foods otherwise low in protein [11,12].

Gliadins are monomeric proteins that can be separated into four groups, alpha-, beta-, gamma- and omega-gliadins. Glutenins occur as multimeric aggregates of high molecular weight (HMW) and low-molecular-weight (LMW) subunits held together

Table 8.3 Chemical composition of Rice husk ask

<table>
<thead>
<tr>
<th>Component</th>
<th>%</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO₂</td>
<td>92.498</td>
</tr>
<tr>
<td>Fe₂O₃</td>
<td>0.136</td>
</tr>
<tr>
<td>Al₂O₃</td>
<td>0.249</td>
</tr>
<tr>
<td>CaO</td>
<td>0.622</td>
</tr>
<tr>
<td>MgO</td>
<td>0.442</td>
</tr>
<tr>
<td>K₂O</td>
<td>2.490</td>
</tr>
<tr>
<td>LOI</td>
<td>3.520</td>
</tr>
<tr>
<td>Na₂O</td>
<td>0.023</td>
</tr>
</tbody>
</table>

Figure 8.3 Structure of wheat gluten husk.
by disulphide bonds. In wheat, omega- and gamma-gliadins are encoded by genes at the Gli-1 loci located on the short arms of group 1 chromosomes, while alpha and beta-gliadin-encoding genes are located on the short arms of group 6 chromosomes. LMW glutenins are encoded by genes at the Glu-3 loci that are closely linked to the Gli-1 loci. HMW glutenins are encoded by genes at the Glu-1 loci found on the long arms of group 1 chromosomes. Each Glu-1 locus consists of two tightly linked genes encoding one ‘x’-type and one ‘y’-type HMW glutenin, with polymorphism giving rise to a number of different alleles at each locus.

The y-type genes at the Glu-A1 locus are not expressed in hexaploid wheat. Due to the very close linkage between the x and y type genes, HMW glutenins are classified into alleles according to the x and y type subunits expressed. Considerable efforts have been made to understand the relationship between gliadin and glutenin composition and rheological properties of wheat dough. It is now well understood that the properties of various wheat storage proteins have a major effect on dough rheological properties.

The gliadin and glutenin components contribute to dough quality either in an independent manner (additive genetic effects) or in interactive manner (epistatic effects). It was suggested that the apparent effects of gliadins on dough quality should be attributed to the LMW glutenins due to the close linkage of the Gli-1 and Glu-3 loci. Generally, HMW glutenins have been found to be more important than gliadins and LMW glutenins for dough rheological properties [14].

8.1.2.2.1 Composition and Properties

a) Film Forming

The film forming property of hydrated wheat gluten is a direct outcome of its viscoelasticity. Whenever carbon dioxide or water vapor forms internally in a gluten mass with sufficient pressure to partially overcome the elasticity, the gluten expands to a spongy cellular structure. In such structures, pockets or voids are created which are surrounded by a continuous protein phase to entrap and contain the gas or vapor. This new shape and structure can then be rendered dimensionally stable by applying sufficient heat to cause the protein to denature or devitalize and set up irreversibly into a fixed moist gel structure or to a crisp fragile state, depending on final moisture content.

The open texture of leavened breads; the suspension of solid particles such as fruit pieces or grains; and high fiber bread are examples of success due to the continuous phase of hydrated protein. Where the loading of added solid particles is greater than the strength possible from the flour used, “cripples” result. This is easily correctable by addition of wheat gluten to the flour base. In addition to its film forming potential in food systems, cast or floated films of wheat gluten can be made. Glazing of meat patties is possible, and wheat gluten films in the form of sausage casing, tubes or shreds are recorded in the patent literature as the product of gluten “hot melt” techniques.

b) Flavor

Properly produced and given reasonable care in storage, wheat gluten exhibits a flavor note variously described as “bland” or “slight cereal.” Wheat gluten flavors enjoy wide acceptance and wheat gluten merges perfectly into all cereal-based products. Blending with meats in various binding, adhesive and extension roles need not result in off-flavor notes, even at high percentage use levels. Blending of wheat gluten with other food
proteins which do possess characteristic flavor notes can result in improved total flavor as, for example, when soy/wheat gluten blends are used for textured vegetable protein manufacture. Low and acceptable flavor levels of wheat gluten are the result of careful selection of flours, good manufacturing procedures and proper storage at normal ambient temperatures.

c) pH Effects
Since wheat gluten is a complex of proteins it has no sharp isoelectric (minimum solubility and dissociation) point. There is thus no readily discernible point at which the positive and negative charges exactly balance. Because glutenin is essentially insoluble in water over normal pH ranges, wheat gluten tends to reflect the isoelectric behavior of gliadin in pH/solubility properties. When gliadin is separately examined for pH/solubility criteria, it displays minimum solubility over the pH range 6–9. It is in this range that the cohesive, extensible network of wheat gluten is strongest. It is important to note that wheat gluten becomes more soluble in acid or alkaline dispersions (Some manufacturers utilize this effect to produce spray dried wheat gluten.

The aqueous acetic acid or ammonia used is flashed off during the drying step, and the powdered material retains typical vital gluten characteristics). pH manipulation may thus provide interesting property variations in wheat gluten containing foods [15].

8.1.3 Benzophenone

Benzophenone is the organic compound with the formula (C₆H₅)₂CO, generally abbreviated Ph₂CO (see Figure 8.4). Benzophenone is a widely used building block in organic chemistry, being the parent diarylketone.

Benzophenone is used as a flavor ingredient, a fragrance enhancer, a perfume fixative and an additive for plastics, coatings and adhesive formulations; it is also used in the manufacture of insecticides, agricultural chemicals, hypnotic drugs, antihistamines and other pharmaceuticals [16].

Benzophenone is used as an ultraviolet (UV)-curing agent in sunglasses, and to prevent UV light from damaging scents and colours in products such as perfumes and soaps. Moreover, it can be added to plastic packaging as a UV blocker, which

Figure 8.4 Benzophenone structure.
allows manufacturers to package their products in clear glass or plastic rather than opaque or dark packaging. It is also used in laundry and household cleaning products. Benzophenone is widely used as a photoinitiator for inks and varnishes that are cured with UV light. In addition to being a drying catalyst, benzophenone is an excellent wetting agent for pigments; it can also be used in printing to improve the rheological properties and increase the flow of inks by acting as a reactive solvent [16,17].

8.1.4 Glibenclamide

Glibenclamide (Figure 8.5) is chemically known as 5-chloro-N-[2-[4[(cyclohexylamino) carbonyl] amino] sulfonyl] phenyl] ethyl]-2-methoxy benzamide is second generation sulphonyl ureas drug widely used in treatment of type 2 diabetic patients. It acts by inhibiting ATP-sensitive potassium channels in pancreatic beta cells causing cell membrane depolarization (increasing intracellular calcium in the beta cell) which stimulates the insulin release [18]. It was developed in 1966 in a cooperative study between Boehringer Mannheim (now part of Roche) and Hoechst (now part of Sanofi-Aventis).

8.1.4.1 Mechanism of Action

The drug works by inhibiting the sulfonylurea receptor 1 (SUR1), the regulatory sub-unit of the ATP-sensitive potassium channels (K\textsubscript{ATP}) in pancreatic beta cells. This inhibition causes cell membrane depolarization opening voltage-dependent calcium channel. This results in an increase in intracellular calcium in the beta cell and subsequent stimulation of insulin release.

After a cerebral ischemic insult the blood brain barrier is broken and glibenclamide can reach the central nervous system. Glibenclamide has been shown to bind more efficiently to the ischemic hemisphere. Moreover, under ischemic conditions SUR1, the regulatory subunit of the K\textsubscript{ATP} and the NC\textsubscript{Ca,ATP} channels, is expressed in neurons, astrocytes, oligodendrocytes, endothelial cells and by reactive microglia.
8.1.4.2 Medical Uses

It is used in the treatment of type 2 diabetes. As of 2011, it is one of only two oral antidiabetics in the World Health Organization Model List of Essential Medicines (the other being metformin). As of 2003, in the United States, it was the most popular sulfonylurea. Additionally, recent research shows that glibenclamide improves outcome in animal stroke models by preventing brain swelling and enhancing neuroprotection. A retrospective study showed that in type 2 diabetic patients already taking glyburide, NIH stroke scale scores on were improved on discharge compared to diabetic patients not taking glyburide [19-21].

8.2 Methodology

8.2.1 Geometry Optimization

In this study the semi-empirical methods were used for describing the potential energy function of the system. Next a minimization algorithm is chosen to find the potential energy minimum corresponding to the lower-energy structure.

Iterations number and convergence level lead optimal structure. The optimizing process of structures used in this work was started using the AMBER/AM1 methods, because it generates a lower-energy structure even when the initial structure is far away from the minimum structure. The Polak-Ribiere algorithm was used for mapping the energy barriers of the conformational transitions. For each structure, 1350 iterations, a level convergence of 0.001 kcal/mol/Å and a line search of 0.1 were carried out [22].

8.2.2 FTIR

The infrared spectrum is commonly obtained by passing infrared electromagnetic radiation through a sample that possesses a permanent or induced dipole moment and determining what fraction of the incident radiation is absorbed at a particular energy [23]. The energy of each peak in an absorption spectrum corresponds to the frequency of the vibration of a molecule part, thus allowing qualitative identification of certain bond types in the sample. The FTIR was obtained by first selecting menu Compute, vibrational, rotational option, once completed this analysis, using the option vibrational spectrum of FTIR spectrum pattern is obtained for two methods of analysis.

8.2.3 Electrostatic Potential

After obtaining a free energy of Gibbs or optimization geometry using AMBER/AM1 methods, we can plot two-dimensional contour diagrams of the electrostatic potential surrounding a molecule, the total electronic density, the spin density, one or more molecular orbitals, and the electron densities of individual orbitals. HyperChem software displays the electrostatic potential as a contour plot when you select the appropriate option in the Contour Plot dialog box. Choose the values for the starting contour
and the contour increment so that you can observe the minimum (typically about -0.5 for polar organic molecules) and so that the zero potential line appears.

A menu plot molecular graph, the electrostatic potential property is selected and then the 3D representation mapped isosurface for both methods of analysis. Atomic charges indicate where large negative values (sites for electrophilic attack) are likely to occur. However, the largest negative value of the electrostatic potential is not necessarily adjacent to the atom with the largest negative charge [24].

8.3 Results and Discussions

8.3.1 Geometry Optimization

The values of different thermodynamic parameters of both lignocellulosic materials are described in Table 8.4. The negative value of ΔG (Gibbs free energy) reflects the spontaneity of materials [25]. Attractive interactions between π systems are one of the principal non-covalent forces governing molecular recognition and play important roles in many chemical systems. Attractive interaction between π systems is the interaction between two or more molecules leading to self-organization by formation of a complex structure which has lower conformation equilibrium than of the separate components and shows different geometrical arrangement with high percentage of yield (Figures 8.6–8.7).

The difference in the energy values are attributed to the constituents of the lignocellulosic material [6]. Log P negative shows that these lignocellulosic materials can absorb polar solvents because of its hydrophilic character characteristic of cellulose [26,27].

8.3.2 FTIR Analysis

Table 8.5 shows the FTIR bands of rice husk where the characteristic peaks associated with organic components are observed. CH asymmetric (5743 cm⁻¹), C = O stretching hemicelluloses (1745 cm⁻¹) [28]. The absorption band at 3387 cm⁻¹ corresponds to the combined bands of the NH₂ and OH group stretching vibration to chitosan [29]. The vibrations of the aromatic rings can be observed at 1846, 1718, 1413 and 1077 cm⁻¹, respectively. At 3125 and 2849 cm⁻¹ were attributed at CH stretching in cellulose-rich material. Both cellulose/hemicelluloses -and lignin- associated bands are present in the

<table>
<thead>
<tr>
<th>Properties</th>
<th>Rice husk</th>
<th>Wheat gluten husk</th>
</tr>
</thead>
<tbody>
<tr>
<td>ΔG (Kcal/mol)</td>
<td>-258.07</td>
<td>-195.25</td>
</tr>
<tr>
<td>Surface area (Å²)</td>
<td>2672.40</td>
<td>1479.34</td>
</tr>
<tr>
<td>Volumen (Å³)</td>
<td>6966.35</td>
<td>2772.21</td>
</tr>
<tr>
<td>Mass (amu)</td>
<td>3468.45</td>
<td>1074.18</td>
</tr>
<tr>
<td>Log P</td>
<td>-22.24</td>
<td>-15.61</td>
</tr>
</tbody>
</table>
Figure 8.6  Rice husk optimum.

Figure 8.7  Wheat gluten husk optimum.
rice husk, and this suggests the presence of lignin-carbohydrate matrix in rice husk. In fact, the band at 815 cm$^{-1}$ shows the strongest absorption. This band corresponds to the CO stretching vibration in both cellulose/hemicellulose and lignin, and it explains the lignocellulosic nature of rice husk [30].

Wheat gluten husk was analyzed using FTIR to know the various chemical constituents present (see Table 8.6). At 5741 cm$^{-1}$ was assigned to NH stretching, from 4279 at 4029 cm$^{-1}$ was attributed to CH stretching, the vibrations of CH$_2$ and NH$_2$ corresponding to 3695 cm$^{-1}$. The band at 3319 cm$^{-1}$ is assignment to hydrogen bonded OH stretching. The hydrophilic tendency of wheat husk was reflected at 3695 cm$^{-1}$ which is related to the OH groups present in aliphatic in this material. The bands in the range 1450–1370 cm$^{-1}$ were assigned from the CH symmetric and asymmetric deformations. The region of 1200–1000 cm$^{-1}$ represents the CH, C–N and C–O stretching and deformation bands in cellulose and lignin [31]. The lignocellulosic material peak corresponds to C = O and C = C bond appears to 3555, 3366 and 3024 cm$^{-1}$ [32]. Finally, the C–C, C–N and C–O bond were observed to 2619 ad 1096 cm$^{-1}$.

Table 8.5 FTIR assignments of rice husk. Table 8.6 FTIR assignments of wheat gluten husk.

8.3.3 Electrostatic Potential

Molecular electrostatic potential (MESP), which is related to the electronegativity and the partial charge changes on the different atoms of the molecule, when plotted on the isodensity surface of the molecule MESP mapping is very useful in the investigation of the molecular structure with its physiochemical property relationships. Red and blue areas in the MESP refer to the regions of negative and positive and correspond to the electron-rich and electron-poor regions, respectively, whereas the green color signifies the neutral electrostatic potential [33]. The MESP in case of Figure 8.8(a) clearly suggest that each C–OH, C–O–C bonds represent the most negative potential region of rice husk with a 0.986 at 0.066 eV. Figure 8.8(b) shows that NH and CH bond present neutral potential electrostatic region, glutenine structure represent the most negative potential region and finally the CH$_2$ and CH represent the most positive potential region. This potential has a value of 1.013 at 0.067 eV.

8.3.4 Absorption of Benzophenone

8.3.4.1 Geometry Optimization

Table 8.7 shows that negative values of $\Delta H$ suggested that the exothermic nature of the adsorption. Negative values of $\Delta G$ indicated the spontaneous nature of the adsorption process of benzophenone [34]. One can see that the properties change with the addition of benzophenone, for example the Log P values in both cases determined that the materials tend to be more negative which found that tend to absorb water (polar solvents) because of its hydrophilic character characteristic of cellulose [26,27]. Figures 8.9–8.10 show the absorption of benzophenone, in where the formation of hydrogen
bonds can be seen after calculating Gibbs free energy, the negative regions were located in the C = C and C–OH bonds respectively.

### 8.3.4.2 FTIR

Table 8.8 shows the FTIR bands of rice husk/benzophenone where the characteristic peaks associated with absorption process are observed. Comparing the results of Tables 8.5 and 8.8, can be seen that there are shifts in the peaks of rice husk attributed to the

---

**Figure 8.8** Electrostatic potential of (a) rice husk and (b) wheat gluten husk, respectively.
absorption of benzophenone, so the existence of one or more aromatic rings in a structure is normally readily determined from the CH and C = C–C ring related vibrations. The CH stretching occurs above 2893 cm⁻¹ and is typically exhibited as a multiplicity of weak to moderate bands, compared with the aliphatic CH stretch [35-37].

<table>
<thead>
<tr>
<th>Properties</th>
<th>Rice husk/ benzophenone</th>
<th>Wheat gluten husk/benzophenone</th>
</tr>
</thead>
<tbody>
<tr>
<td>ΔG (Kcal/mol)</td>
<td>-190</td>
<td>- 55.68</td>
</tr>
<tr>
<td>Surface area (Å²)</td>
<td>2952.04</td>
<td>2395.89</td>
</tr>
<tr>
<td>Volumen (Å³)</td>
<td>7973.28</td>
<td>4409.02</td>
</tr>
<tr>
<td>Mass (amu)</td>
<td>4014.10</td>
<td>1620.84</td>
</tr>
<tr>
<td>Log P</td>
<td>-27.18</td>
<td>-24.25</td>
</tr>
</tbody>
</table>

Figure 8.9  Rice husk/benzophenone structure after Gibbs free energy.

Figure 8.10  Wheat gluten husk/benzophenone structure after Gibbs free energy.
characteristic infrared absorption frequencies of carbonyl group in cyclic ketones are normally strong in intensity and found in the region 1585–1621 cm$^{-1}$. The interaction of carbonyl group with other groups present in the system did not produce such a drastic and characteristic change in the frequency of C = O stretch as did by interaction of NH stretch. The carbon–oxygen double bond is formed by pπ–pπ between carbon and oxygen. Because of the different electronegativities of carbon and oxygen atoms, the bonding electrons are not equally distributed between the two atoms. The lone pair of electrons on oxygen also determines the nature of the carbonyl group. The position of the C = O stretching vibration is very sensitive to various factors such as the physical state, electronic effects by substituents, ring strains. Normally carbonyl group vibrations occur in the region 1770 and 1685 cm$^{-1}$. The band at 1482 cm$^{-1}$ is due to C = O stretching vibration of carbonyl group (benzophenone).

While that the Table 8.9 shows the FTIR bands of wheat gluten husk/benzophenone where the characteristic peaks associated with absorption process are observed. The NH and CH stretching modes arising from amino groups appear around 5749 and 3502 cm$^{-1}$. The stretching modes of NH$_2$ group were assigned to the bands at 6111 cm$^{-1}$[31, 36]. The aromatic CH stretching vibrations appear weak just above 4564 cm$^{-1}$. A highly intense and well defined peak observed at 3258, 2853 cm$^{-1}$ is due to the C = O stretching vibration of carbonyl group (benzophenone).

The C = C vibrations of aromatic ring are confirmed at 3725, 3677 and 3234 cm$^{-1}$. The group of bands at 1792 and 691 cm$^{-1}$ is due to aromatic CH bends [38].

### Table 8.8 FTIR of rice husk/benzophenone.

<table>
<thead>
<tr>
<th>Assignments</th>
<th>Wavenumber (cm$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>C–H asymmetric stretching (rice husk)</td>
<td>5662</td>
</tr>
<tr>
<td>CH$_2$ asymmetric stretching (rice husk)</td>
<td>5492</td>
</tr>
<tr>
<td>C = C (rice husk)</td>
<td>3810, 3724, 3653</td>
</tr>
<tr>
<td>CH = CH (rice husk)</td>
<td>3260</td>
</tr>
<tr>
<td>C–H (rice husk)</td>
<td>3038</td>
</tr>
<tr>
<td>C–H (benzophenone)</td>
<td>2893</td>
</tr>
<tr>
<td>C = O (rice husk)</td>
<td>2858</td>
</tr>
<tr>
<td>C–H</td>
<td>2678, 2367</td>
</tr>
<tr>
<td>C–C scissoring</td>
<td>2026, 869</td>
</tr>
<tr>
<td>C–C, C–O (rice husk)</td>
<td>1843, 1008</td>
</tr>
<tr>
<td>C = O (benzophenone)</td>
<td>1770, 1685</td>
</tr>
<tr>
<td>Ketone</td>
<td>1585, 1621</td>
</tr>
<tr>
<td>C–O, C–H (rice husk)</td>
<td>1610</td>
</tr>
<tr>
<td>C–C stretching (benzophenone)</td>
<td>1482</td>
</tr>
<tr>
<td>C–H (benzophenone)</td>
<td>1416</td>
</tr>
<tr>
<td>C–H (benzophenone), C–C and C–O (rice husk)</td>
<td>1326</td>
</tr>
</tbody>
</table>
8.3.4.3 Electrostatic Potential

The electrostatic potential of rice husk and wheat gluten husk with benzophenone can be observed in Figure 8.11. The results show that the negative (red) regions of MESP were related to electrophilic reactivity and the positive (blue) regions to nucleophilic reactivity. The negative regions are mainly localized on the C = O bond. Also, a negative electrostatic potential region is observed around the OH groups (oxygen atom) [35]. The values of the Figures 8.8–8.9 show that the electronegativity of the benzophenone produces a decrease in nucleophilic areas (blue) of both lignocellulosic materials.

8.3.5 Absorption of Glibenclamide

8.3.5.1 Geometry Optimization

Structural properties of rice husk and wheat gluten husk with glibenclamide are listed in Table 8.10 where the Gibbs free energy is spontaneous for both lignocellulosic materials. The solubility of glibenclamide is an important factor in determining the rate and extent of its absorption process [39]. The computed Log P values (P is the partition coefficient of the molecule in the water–octanol system), show that the absorption is effected due to the hydrophilic character and additionally the absorption plays an important role in both partition and receptor binding processes of drug action. Drug design is an iterative process which begins with a compound that displays an interesting biological profile and ends with optimizing both the activity profile for the molecule and its chemical synthesis. It is therefore, important to know if drug molecules exist predominantly in the basic or protonated forms [40]. Rice husk/glibenclamide and wheat gluten husk/glibenclamide structure are appreciated in Figure 8.12, where it
observed that the glibenclamide is absorbed through the formation of hydrogen bonds between C = O, NH, C–O and CH bonds.

8.3.5.2 FTIR

In the FTIR results of rice husk/glibenclamide can be seen in Table 8.11, the principal absorption peaks appeared at 5505 cm⁻¹ was attributed to CH₃ stretching, at 3368 cm⁻¹ due to the NH stretching, the absorption of C = O and S = O were observed at 1549 cm⁻¹[41]. In the rice husks, the band at 3754 cm⁻¹ is representative of the CH and OH
bonds. Both bands are ascribed to the stretching of hydrogen bonds and bending of hydroxyl (OH) groups bound to the cellulose structure. The absorption phenomenon was observed at 2412 and 793 cm⁻¹ refers to the bending frequency of C–C, CH, C–O and OH respectively, while the absorption around 1955, 1334, 1090 and 924 cm⁻¹ were refers to the C–C and C–O of the cellulose component. The results indicate that the glibenclamide was absorbed by rice husk [42]. Table 8.12 shows FTIR results of wheat gluten husk/glibenclamide where, the first characteristic peak appears at 5879 cm⁻¹ as a result of C–H and O–H stretching, indicating the presence of bonded hydroxyl groups in the molecular structure of glutenin (wheat husk) [43]. Between 5007 and 5583 cm⁻¹ are principally attributed to NH and CH asymmetric stretching vibrations of glibenclamide. The peaks characteristics of glibenclamide were observed to 4511, 4028 and 3529 cm⁻¹ and attributed to CH₂ stretching, CH₃ (O-CH₃) and CH = CH, respectively. The wheat gluten husk components were assigned to 3392, 2022, 1739 and 819 cm⁻¹.

Figure 8.12 Glibenclamide absorption structure, (a) Rice husk (b) Wheat gluten husk structure, respectively.
8.3.5.3 Electrostatic Potential

Figure 8.13 shows the rice husk/glibenclamide and wheat gluten husk/glibenclamide MESP, where can be observed that the values are very similar at lignocellulosic materials (see Figure 8.8). The negative regions were appreciated at OH groups (C–OH bonds). The absorption of the glibenclamide can be seen mainly in to the rice husk by the formation of hydrogen bonds between the OH and NH, respectively.

Table 8.11 FTIR results of Rice husk/glibenclamide

<table>
<thead>
<tr>
<th>Assignments</th>
<th>Wavenumber (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH₃ stretching (O-CH₃ glibenclamide)</td>
<td>5505</td>
</tr>
<tr>
<td>CH, O–H (rice husk)</td>
<td>3754</td>
</tr>
<tr>
<td>C = C (rice husk)</td>
<td>3640, 3506</td>
</tr>
<tr>
<td>NH stretching (glibenclamide)</td>
<td>3368</td>
</tr>
<tr>
<td>CH scissoring (rice husk)</td>
<td>3166</td>
</tr>
<tr>
<td>C = C (rice husk)</td>
<td>2986</td>
</tr>
<tr>
<td>C–C (rice husk)</td>
<td>2709</td>
</tr>
<tr>
<td>C–C, C–H and C–O (rice husk)C–C, C–H (glibenclamide)</td>
<td>2412</td>
</tr>
<tr>
<td>C–C, C–O (rice husk)</td>
<td>1955, 1334, 1090, 924</td>
</tr>
<tr>
<td>C–C, C–N, C–H (rice husk)</td>
<td>1758</td>
</tr>
<tr>
<td>C = O, S = O (glibenclamide)</td>
<td>1549</td>
</tr>
<tr>
<td>O–H, C–H (rice husk)</td>
<td>695</td>
</tr>
</tbody>
</table>

Table 8.12 FTIR results of Wheat gluten husk/glibenclamide

<table>
<thead>
<tr>
<th>Assignments</th>
<th>Wavenumber (cm⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>CH, O–H asymmetric stretching (glutenin: wheat gluten husk)</td>
<td>5879</td>
</tr>
<tr>
<td>NH asymmetric stretching (glibenclamide)</td>
<td>5583</td>
</tr>
<tr>
<td>CH asymmetric stretching (glibenclamide)</td>
<td>5007</td>
</tr>
<tr>
<td>CH₂ stretching (glibenclamide)</td>
<td>4511</td>
</tr>
<tr>
<td>CH₃ (O-CH₃: glibenclamide)</td>
<td>4028</td>
</tr>
<tr>
<td>CH = CH (glibenclamide)</td>
<td>3529</td>
</tr>
<tr>
<td>CH (gliadin: wheat gluten husk)</td>
<td>3392</td>
</tr>
<tr>
<td>C = C (ring: glibenclamide)</td>
<td>2830</td>
</tr>
<tr>
<td>C = C, C = O, S = O</td>
<td>2474</td>
</tr>
<tr>
<td>C–C, C–H, C–O (glutenin: wheat gluten husk)</td>
<td>2022</td>
</tr>
<tr>
<td>CH deformation (glutenin: wheat gluten husk)</td>
<td>1739</td>
</tr>
<tr>
<td>C–C, C–N, C–O (glibenclamide)</td>
<td>1332, 1124, 1028, 569</td>
</tr>
<tr>
<td>C–C, C–N, C–O (gliadin: wheat gluten husk)</td>
<td>819</td>
</tr>
</tbody>
</table>

8.3.5.3 Electrostatic Potential

Figure 8.13 shows the rice husk/glibenclamide and wheat gluten husk/glibenclamide MESP, where can be observed that the values are very similar at lignocellulosic materials (see Figure 8.8). The negative regions were appreciated at OH groups (C–OH bonds). The absorption of the glibenclamide can be seen mainly in to the rice husk by the formation of hydrogen bonds between the OH and NH, respectively.
8.4 Conclusions

The rice husks and wheat gluten husk on an individual basis and such as benzophenone and glibenclamide absorption systems were analyzed to determine the applications of lignocellulosic materials. It was determined that the negative value of the ΔG verifies that the absorption process is carried out in a way spontaneous. The negative values of Log P show that the absorption is affected due to the hydrophilic character and additionally the absorption plays an important role in both partition and receptor binding processes of absorption (benzophenone and glibenclamide). FTIR results show that there are shifts in the peaks of rice husk and wheat gluten husk attributed to the absorption of benzophenone and glibenclamide. The MESP values indicated the nucleophilic and electrophilic regions mainly in the NH, C-O and C = O bonds respectively.

Figure 8.13 MESP of (a) Rice husk/glibenclamide, (b) wheat gluten husk/glibenclamide.
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34. Z. Xi-Ming, and F. Rong-Yu, Solid flux of pulverized coal of high-pressure and dense-phase pneumatic conveying and ANN simulation. *CIESC J.* 64(5), 0-0 (2013).


