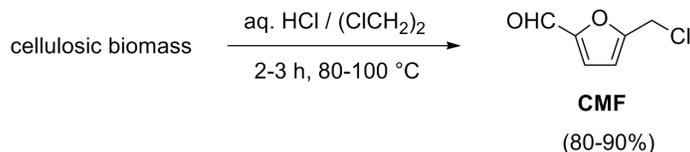


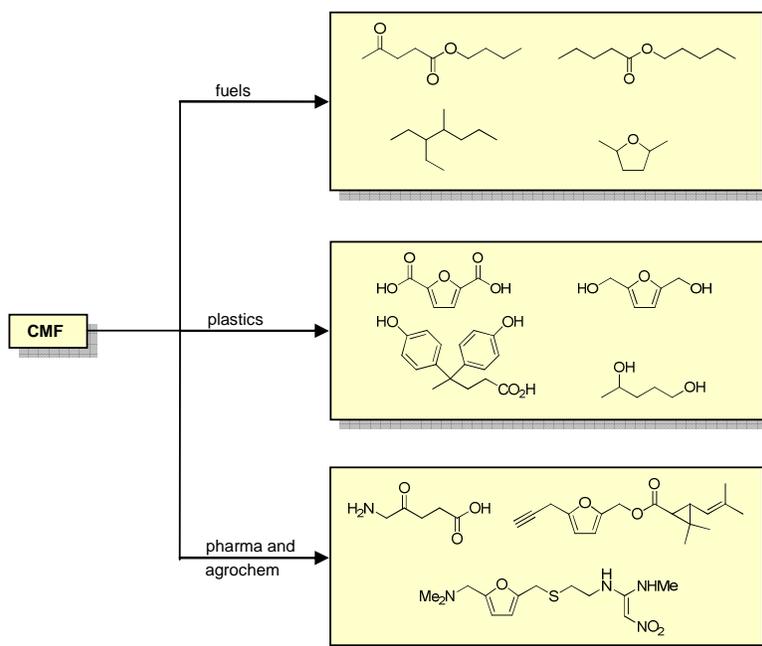
## Project Statement – M. Mascal, University of California Davis

**Background:** We are developing a novel technology to efficiently convert waste biomass (agricultural, municipal, forestry) into biofuels and value-added products. The process involves the acidic digestion of the carbohydrate content of biomass (sugars, starch, polysaccharides) in a biphasic reactor under mild conditions (80 °C, 2-3 h) to give 5-(chloromethyl)furfural (CMF) as the main product in isolated yields of 80-90%.<sup>[1]-[3]</sup>



The characteristics of the process can be summarized as follows:

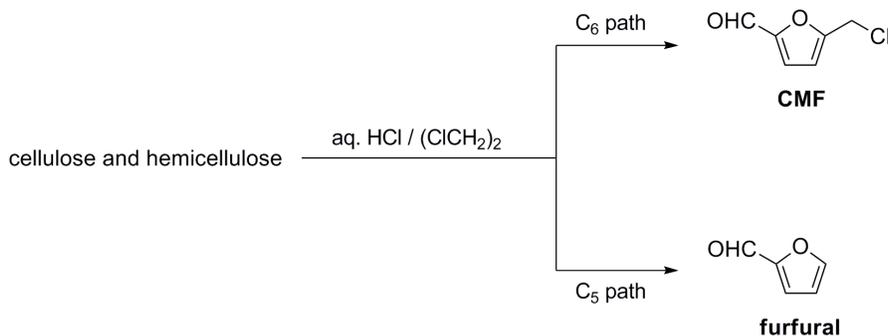
1) *The product is commercially versatile.* CMF is an emerging, renewable platform chemical which provides access to a versatile portfolio of products that originate from either a substituted furan or levulinic acid derivative manifold. The production of CMF can be coupled with that of biodiesel from oil-seed feedstocks,<sup>[4]</sup> or applied to the synthesis of stand-alone fuels which are high-energy, hydrophobic, non-corrosive, sulfur-free, low-toxicity organic liquids compatible with the existing automotive infrastructure. CMF derivatives also span a range of specialty chemical markets, including monomers for renewable polymers, pharmaceuticals, and agrochemicals (shown below).<sup>[5]-[9]</sup>



2) *The yield is extraordinary.* We know of no other biomass conversion process that gives such high isolated yields of simple organic products from cellulosic sources.

3) *The process is completely chemical in nature and operates under mild conditions.* No expensive catalysts, enzymes, microorganisms, or extremes in temperature or pressure are involved.

4) *It features the total carbohydrate utilization of biomass, with 100% carbon efficiency.* The C<sub>6</sub> (cellulose) and C<sub>5</sub> (hemicellulose) streams are co-harvested to give C<sub>6</sub> and C<sub>5</sub> furanic products, as shown below. No carbons are sacrificed in the process, and there is no waste stream.<sup>[10]</sup>



5) *Mixed lignocellulosic biomass can be directly utilized with minimal pretreatment.* The process is feedstock agnostic, and only mechanical reduction of bulk biomass into particles is required. Since the process is aqueous, even drying of the substrate is not necessary.

6) *It represents an innovation in the area of biomass valorization.* To date, no other reported technology centers on CMF as a biomass-derived intermediate for biofuel and value-added material production.

**Research Project:** The proposed duration of the project is one 20-week semester, although it is possible that a two-semester stay could be arranged (this would have to be determined if the application is successful). As such, a realistic plan of projects that can be initiated and progressed to some extent within that time frame is described below. It is anticipated that continued collaboration in the period after the visit would see the conclusion of any unfinished activities. Research will involve partnering with chemical and environmental engineers in the Department of Energy and Environment at Chalmers University of Technology in Göteborg to work on the implementation of the above described technology by performing an integrated, system-level conceptual process model on the production scale, including block and process flow diagrams, mass and energy balances, and cost analysis. The proposed outcomes will be the following:

1) *The development of reactor models.* We will work to develop fundamental reactor models for CMF production. This modeling presents unique challenges due to two-phase characteristics of the reaction mixture. The developed models will allow us to study various reactor configurations and recycle and feed strategies. The initial focus, for simplicity, will be on continuous stirred tank reactors (CSTRs) for this liquid phase reaction, and design parameters such as residence times, solvent/feed ratios, and temperature will be explored in terms of their impact on conversion, product selectivity, and energy requirements. The simulation platform will enable us

to carry out sensitivity studies as well as rigorous optimizations to determine best operating conditions.

2) *Reactor sequencing and design of separation tasks.* A key element of the process to produce CMF is the separation and recovery of various components. These design decisions will generate a number of alternatives that can be best evaluated using simulation platforms and will involve the sequence of separation tasks that follow the CMF reactor, and more critically subsequent reactors that convert CMF into marketable derivatives, separating products from any by-products and unconverted reactants in an economically and technically feasible manner. The order with which the components are recovered from a mixture is very important for cost calculations. The sequencing of recovery units generates alternatives that need to be evaluated using heuristic and rigorous criteria. Furthermore, the operating conditions for each unit need to be determined individually so that capital and operating costs can be incorporated into the design decision-making.

3) *Flowsheet simulations.* The simulations of the flowsheet that include all tasks will enable an in-depth study of process strategies. It is noted that the technology proposed here is inherently waste free, yet unconvertible side products (e.g. lignin) can be introduced with various feed streams. The possible origin and destination of such side products will be evaluated to ensure any waste/unwanted material is explicitly accounted for in the flowsheet and also to determine its quantity and impact on the economics of the process. A key outcome of the proposed work will be a detailed process flow diagram that will describe a complete arrangement of process units to enable the production of the products in a technically feasible and economical manner.

4) *Environmental modeling.* This will involve preliminary environmental performance modeling, feedstock availability/sourcing analysis, and plans for pre-market product education/acceptance activities.

5) *Biofuel characterization and combustion tests.* This activity will include the measurement of fuel specifications<sup>[11]</sup> and combustion performance of novel furanic and levulinic-based biofuels derived from CMF.

6) *Mass transfer study.* Finally, if time permits, a biomass to CMF reactor can be set up to study mass transfer limitations with respect to particle size. The reaction-extraction phenomena in a continuously stirred reactor are complex. The problem here is one of mass transfer in a medium involving aqueous acid, microcrystallites of cellulose and organic solvent. Some of the fundamental issues that could be addressed are the determination of the minimum agitation speed for complete dispersion of the solvent and biomass particles, and mass transfer characterization and the elimination of mass transfer limitations in the aqueous acid phase.

The above project will prove to be excellent research opportunity for a graduate student in the host institution to study and model a novel biorefinery technology.

**Relevance to Host Country:** This technology is of particular relevance to Sweden and the Scandinavian countries in general, with their extensive forestry biomass resources and strong emphasis on environmental conservation and management, so there is much to be gained in the

course of this collaboration. Opportunities for broader collaboration on biomass-based fuel and chemical projects within Scandinavia will also be explored.

**Teaching:** I plan to deliver a graduate course on the chemistry of energy technologies, which will include the basic economics of energy production, fossil fuels, petrochemicals, and alternative energies (geothermal, solar, wind, hydroelectric, ocean energy conversion, and fermentative, thermochemical, and chemical biomass-based approaches), in addition to the development of hypothetical alternative energy economies (hydrogen, methanol). A syllabus that includes this material is uploaded as an attachment to the application.

I have taught chemistry courses at the graduate and undergraduate levels for about 20 years, and recently have begun to incorporate aspects of renewable energy science into the chemistry curriculum here at UC Davis.<sup>[12]</sup> My preparation to teach outside the US is very substantial in that I did my Ph.D. in London and was an academician in the United Kingdom (University of Nottingham) for several years before returning to the US. I have traveled extensively in Scandinavia (in my formative years) and have a keen appreciation for its culture. Finally, I have also studied (postdoctoral research) in France with Nobel Prize winner Jean-Marie Lehn. Having thus traveled widely on the European continent, I am well calibrated to the pedagogical style of its educational systems. All the same, not having actually taught a course in Sweden, I anticipate that the experience will be a mutually enriching one for myself, the faculty at Chalmers University, and the students.